Table 1. Positional parameters and B(eq) for **2**.

atom	x	y	z	B(eq)
Ir(1)	0.55639(4)	0.22378(3)	0.23780(3)	1.475(8)
P(1)	0.4397(2)	0.22937(18)	0.09334(14)	1.52(5)
P(2)	0.3692(2)	0.1547(2)	0.26078(15)	1.58(5)
P(3)	0.5794(2)	0.4006(2)	0.28084(15)	1.59(5)
O(1)	1.0239(8)	0.1341(7)	0.5850(5)	6.1292
C(1)	0.7435(8)	0.2431(8)	0.2234(6)	1.9936
C(2)	0.6448(7)	0.1395(7)	0.1816(6)	1.4148
C(3)	0.5853(8)	0.0648(7)	0.2290(6)	1.7738
C(4)	0.6576(8)	0.0390(8)	0.3160(6)	2.5369
C(5)	0.7586(9)	-0.0031(8)	0.3092(6)	2.8501
C(6)	0.8449(9)	0.0598(8)	0.2626(6)	3.1362
C(7)	0.9239(8)	0.1830(8)	0.2978(6)	2.5499
C(8)	0.8532(7)	0.2568(7)	0.3052(6)	2.0851
C(9)	0.5259(7)	0.2693(7)	0.0194(5)	1.2875
C(10)	0.6116(8)	0.3779(8)	0.0330(6)	2.2949
C(11)	0.6759(8)	0.4154(7)	-0.0207(5)	1.9823
C(12)	0.6591(8)	0.3462(8)	-0.0892(6)	2.1385
C(13)	0.5760(8)	0.2378(8)	-0.1058(6)	2.4218
C(14)	0.5096(8)	0.1996(7)	-0.0518(6)	1.7945
C(15)	0.3125(7)	0.1001(7)	0.0295(5)	1.4722
C(16)	0.3321(8)	0.0030(7)	0.0285(6)	1.9038
C(17)	0.2373(8)	-0.0972(7)	-0.0195(6)	1.9290
C(18)	0.1214(8)	-0.0993(7)	-0.0669(6)	2.5094
C(19)	0.0999(8)	-0.0039(7)	-0.0678(6)	2.1057
C(20)	0.1950(8)	0.0958(7)	-0.0200(5)	1.9346
C(21)	0.3665(7)	0.3271(7)	0.0939(5)	1.3997
C(22)	0.2976(8)	0.0058(7)	0.2421(6)	1.9027
C(23)	0.3461(8)	-0.0526(8)	0.3037(6)	2.6249
C(24)	0.2984(9)	-0.1655(8)	0.2925(7)	2.8666
C(25)	0.2007(9)	-0.2271(8)	0.2174(7)	3.1438
C(26)	0.1509(8)	-0.1731(7)	0.1574(6)	2.3768
C(27)	0.1977(8)	-0.0592(7)	0.1698(6)	2.1461
C(28)	0.3723(8)	0.1818(7)	0.3703(6)	1.6932
C(29)	0.2586(8)	0.1423(8)	0.3865(6)	2.4281
C(30)	0.2575(9)	0.1569(8)	0.4670(6)	3.0350
C(31)	0.3660(10)	0.2080(8)	0.5360(6)	3.0311
C(32)	0.4788(9)	0.2485(8)	0.5224(6)	2.8318
C(33)	0.4821(8)	0.2336(7)	0.4407(6)	2.1802
C(34)	0.2540(7)	0.2038(7)	0.1966(5)	1.8680
C(35)	0.6687(7)	0.4589(7)	0.3947(5)	1.7776
C(36)	0.6318(8)	0.5213(8)	0.4407(6)	2.3522
C(37)	0.7019(9)	0.5666(8)	0.5258(6)	2.8608
C(38)	0.8118(9)	0.5507(8)	0.5661(6)	2.9365
C(39)	0.8509(8)	0.4904(8)	0.5223(6)	2.7317
C(40)	0.7780(8)	0.4416(7)	0.4372(6)	2.0529
C(41)	0.6702(8)	0.5129(7)	0.2371(5)	1.6749
C(42)	0.7921(8)	0.5231(7)	0.2443(5)	1.8415
C(43)	0.8669(8)	0.6085(8)	0.2159(6)	2.3223
C(44)	0.8229(8)	0.6861(7)	0.1800(6)	2.3569
C(45)	0.7028(9)	0.6762(8)	0.1724(6)	2.5828

atom	x	y	z	B(eq)
C(46)	0.6297(8)	0.5914(7)	0.2013(5)	1.8160
C(47)	0.4299(8)	0.4112(7)	0.2612(6)	1.7666
C(48)	0.1986(7)	0.3723(6)	0.1501(5)	1.3922
C(49)	0.1769(8)	0.4237(8)	0.2140(6)	2.3453
C(50)	0.0753(8)	0.4539(7)	0.1994(6)	2.3590
C(51)	-0.0100(8)	0.4350(7)	0.1161(6)	2.1164
C(52)	0.0108(8)	0.3861(7)	0.0517(5)	1.8607
C(53)	0.1107(7)	0.3538(7)	0.0666(5)	1.8(2)
C(54)	0.8934(14)	0.1455(11)	0.5995(12)	9.0(5)
C(55)	0.8563(11)	0.2355(12)	0.5575(7)	3.6(3)
C(56)	0.9289(16)	0.2719(13)	0.5320(10)	7.2(5)
C(57)	1.0471(13)	0.2537(11)	0.5597(8)	6.1(4)
B(1)	0.3132(9)	0.3295(8)	0.1741(6)	1.4(2)

Table 2. Intramolecular Distances Involving the Nonhydrogen Atoms of **2**.

atom	atom	distance	atom	atom	distance
Ir(1)	P(1)	2.409(2)	C(9)	C(14)	1.40(1)
Ir(1)	P(2)	2.304(2)	C(10)	C(11)	1.37(1)
Ir(1)	P(3)	2.311(2)	C(11)	C(12)	1.35(1)
Ir(1)	C(1)	2.302(9)	C(12)	C(13)	1.38(1)
Ir(1)	C(2)	2.176(8)	C(13)	C(14)	1.39(1)
Ir(1)	C(3)	2.261(9)	C(15)	C(16)	1.39(1)
P(1)	C(9)	1.844(8)	C(15)	C(20)	1.39(1)
P(1)	C(15)	1.841(8)	C(16)	C(17)	1.40(1)
P(1)	C(21)	1.819(8)	C(17)	C(18)	1.38(1)
P(2)	C(22)	1.813(9)	C(18)	C(19)	1.38(1)
P(2)	C(28)	1.841(9)	C(19)	C(20)	1.40(1)
P(2)	C(34)	1.821(8)	C(21)	B(1)	1.67(1)
P(3)	C(35)	1.841(9)	C(22)	C(23)	1.42(1)
P(3)	C(41)	1.842(9)	C(22)	C(27)	1.39(1)
P(3)	C(47)	1.810(8)	C(23)	C(24)	1.38(1)
O(1)	C(54)	1.74(1)	C(24)	C(25)	1.40(1)
O(1)	C(57)	1.60(1)	C(25)	C(26)	1.37(1)
C(1)	C(2)	1.43(1)	C(26)	C(27)	1.39(1)
C(1)	C(8)	1.53(1)	C(28)	C(29)	1.42(1)
C(2)	C(3)	1.43(1)	C(28)	C(33)	1.39(1)
C(3)	C(4)	1.57(1)	C(29)	C(30)	1.36(1)
C(4)	C(5)	1.56(1)	C(30)	C(31)	1.37(1)
C(5)	C(6)	1.53(1)	C(31)	C(32)	1.39(1)
C(6)	C(7)	1.54(1)	C(32)	C(33)	1.39(1)
C(7)	C(8)	1.54(1)	C(34)	B(1)	1.67(1)
C(9)	C(10)	1.40(1)	C(35)	C(36)	1.39(1)
C(35)	C(40)	1.41(1)			
C(36)	C(37)	1.39(1)			
C(37)	C(38)	1.40(1)			
C(38)	C(39)	1.36(1)			
C(39)	C(40)	1.40(1)			
C(41)	C(42)	1.41(1)			
C(41)	C(46)	1.38(1)			
C(42)	C(43)	1.38(1)			
C(43)	C(44)	1.39(1)			
C(44)	C(45)	1.39(1)			
C(45)	C(46)	1.37(1)			
C(47)	B(1)	1.67(1)			
C(48)	C(49)	1.39(1)			
C(48)	C(53)	1.42(1)			
C(48)	B(1)	1.64(1)			
C(49)	C(50)	1.39(1)			
C(50)	C(51)	1.40(1)			
C(51)	C(52)	1.37(1)			
C(52)	C(53)	1.39(1)			
C(54)	C(55)	1.54(2)			
C(55)	C(56)	1.07(2)			
C(56)	C(57)	1.48(2)			

Distances are in angstroms. Estimated standard deviations in the least significant figure are given in parentheses.

Table 3. Intramolecular Bond Angles Involving the Nonhydrogen Atoms of **3**.

atom	atom	atom	angle	atom	atom	atom	angle
P(1)	Ir(1)	P(2)	87.96(8)	C(28)	P(2)	C(34)	104.1(4)
P(1)	Ir(1)	P(3)	90.31(8)	Ir(1)	P(3)	C(35)	116.3(3)
P(1)	Ir(1)	C(1)	99.6(2)	Ir(1)	P(3)	C(41)	118.2(3)
P(1)	Ir(1)	C(2)	86.1(2)	Ir(1)	P(3)	C(47)	112.0(3)
P(1)	Ir(1)	C(3)	104.7(2)	C(35)	P(3)	C(41)	97.3(4)
P(2)	Ir(1)	P(3)	90.11(8)	C(35)	P(3)	C(47)	104.8(4)
P(2)	Ir(1)	C(1)	163.1(2)	C(41)	P(3)	C(47)	106.5(4)
P(2)	Ir(1)	C(2)	129.9(2)	C(54)	O(1)	C(57)	83.4(8)
P(2)	Ir(1)	C(3)	97.5(2)	Ir(1)	C(1)	C(2)	66.7(5)
P(3)	Ir(1)	C(1)	104.9(2)	Ir(1)	C(1)	C(8)	117.2(6)
P(3)	Ir(1)	C(2)	139.6(2)	C(2)	C(1)	C(8)	123.0(8)
P(3)	Ir(1)	C(3)	163.4(2)	Ir(1)	C(2)	C(1)	76.3(5)
C(1)	Ir(1)	C(2)	37.0(3)	Ir(1)	C(2)	C(3)	74.5(5)
C(1)	Ir(1)	C(3)	66.0(3)	C(1)	C(2)	C(3)	120.9(8)
C(2)	Ir(1)	C(3)	37.5(3)	Ir(1)	C(3)	C(2)	68.0(5)
Ir(1)	P(1)	C(9)	117.8(2)	Ir(1)	C(3)	C(4)	115.4(6)
Ir(1)	P(1)	C(15)	117.1(3)	C(2)	C(3)	C(4)	124.0(7)
Ir(1)	P(1)	C(21)	109.6(3)	C(3)	C(4)	C(5)	112.5(7)
C(9)	P(1)	C(15)	100.0(4)	C(4)	C(5)	C(6)	117.5(7)
C(9)	P(1)	C(21)	105.4(4)	C(5)	C(6)	C(7)	117.2(8)
C(15)	P(1)	C(21)	105.6(4)	C(6)	C(7)	C(8)	117.3(7)
Ir(1)	P(2)	C(22)	113.7(3)	C(1)	C(8)	C(7)	113.8(7)
Ir(1)	P(2)	C(28)	117.8(3)	P(1)	C(9)	C(10)	118.6(6)
Ir(1)	P(2)	C(34)	113.0(3)	P(1)	C(9)	C(14)	124.8(6)
C(22)	P(2)	C(28)	99.0(4)	C(10)	C(9)	C(14)	116.6(8)
C(22)	P(2)	C(34)	107.8(4)	C(9)	C(10)	C(11)	122.3(8)
C(10)	C(11)	C(12)	120.1(8)	C(30)	C(31)	C(32)	118.8(9)
C(11)	C(12)	C(13)	120.2(8)	C(31)	C(32)	C(33)	120.5(9)
C(12)	C(13)	C(14)	119.9(8)	C(28)	C(33)	C(32)	121.0(8)
C(9)	C(14)	C(13)	120.9(8)	P(2)	C(34)	B(1)	115.1(6)
P(1)	C(15)	C(16)	120.3(6)	P(3)	C(35)	C(36)	121.7(6)
P(1)	C(15)	C(20)	121.9(6)	P(3)	C(35)	C(40)	120.3(7)
C(16)	C(15)	C(20)	117.7(8)	C(36)	C(35)	C(40)	118.1(8)
C(15)	C(16)	C(17)	121.9(8)	C(35)	C(36)	C(37)	120.8(8)
C(16)	C(17)	C(18)	119.1(8)	C(36)	C(37)	C(38)	120.1(8)
C(17)	C(18)	C(19)	120.2(8)	C(37)	C(38)	C(39)	120.4(8)
C(18)	C(19)	C(20)	120.4(8)	C(38)	C(39)	C(40)	119.5(8)
C(15)	C(20)	C(19)	120.6(8)	C(35)	C(40)	C(39)	121.0(8)
P(1)	C(21)	B(1)	114.7(6)	P(3)	C(41)	C(42)	118.0(6)
P(2)	C(22)	C(23)	119.5(7)	P(3)	C(41)	C(46)	124.5(6)
P(2)	C(22)	C(27)	125.2(7)	C(42)	C(41)	C(46)	117.5(8)
C(23)	C(22)	C(27)	115.3(8)	C(41)	C(42)	C(43)	120.7(8)
C(22)	C(23)	C(24)	122.5(9)	C(42)	C(43)	C(44)	120.2(8)
C(23)	C(24)	C(25)	120.0(9)	C(43)	C(44)	C(45)	119.4(8)
C(24)	C(25)	C(26)	118.8(9)	C(44)	C(45)	C(46)	119.8(8)
C(25)	C(26)	C(27)	120.9(9)	C(41)	C(46)	C(45)	122.4(8)
C(22)	C(27)	C(26)	122.5(8)	P(3)	C(47)	B(1)	115.5(5)
P(2)	C(28)	C(29)	119.4(7)	C(49)	C(48)	C(53)	115.5(7)
P(2)	C(28)	C(33)	123.6(6)	C(49)	C(48)	B(1)	120.4(8)
C(29)	C(28)	C(33)	116.8(8)	C(53)	C(48)	B(1)	124.0(7)
C(28)	C(29)	C(30)	121.2(9)	C(48)	C(49)	C(50)	123.7(8)
C(29)	C(30)	C(31)	121.6(9)	C(49)	C(50)	C(51)	119.6(8)

atom	atom	atom	angle	atom	atom	atom	angle
C(50)	C(51)	C(52)	117.7(8)				
C(51)	C(52)	C(53)	122.6(8)				
C(48)	C(53)	C(52)	120.9(8)				
O(1)	C(54)	C(55)	114.5(9)				
C(54)	C(55)	C(56)	102(1)				
C(55)	C(56)	C(57)	122(1)				
O(1)	C(57)	C(56)	111(1)				
C(21)	B(1)	C(34)	111.3(7)				
C(21)	B(1)	C(47)	109.6(6)				
C(21)	B(1)	C(48)	112.1(7)				
C(34)	B(1)	C(47)	108.9(7)				
C(34)	B(1)	C(48)	105.4(6)				
C(47)	B(1)	C(48)	109.4(7)				

Angles are in degrees. Estimated standard deviations in the least significant figure are given in parentheses.

Table 4. Anisotropic Displacement Parameters for **2**.

atom	U11	U22	U33	U12	U13	U23
Ir(1)	0.01476(18)	0.0199(2)	0.0223(2)	0.00836(14)	0.00572(14)	0.00476(1
P(1)	0.0162(12)	0.0202(13)	0.0233(14)	0.0078(11)	0.0083(11)	0.0047(1
P(2)	0.0186(13)	0.0195(14)	0.0221(14)	0.0084(11)	0.0062(11)	0.0050(1
P(3)	0.0161(13)	0.0223(14)	0.0199(14)	0.0080(11)	0.0030(11)	0.0016(1
O(1)	0.0883	0.0795	0.0951	0.0375	0.0645	0.0258
C(1)	0.0258	0.0346	0.0196	0.0191	0.0054	0.0020
C(2)	0.0114	0.0148	0.0233	-0.0001	0.0068	0.0011
C(3)	0.0145	0.0172	0.0312	0.0054	0.0030	0.0050
C(4)	0.0292	0.0354	0.0393	0.0150	0.0177	0.0165
C(5)	0.0422	0.0424	0.0384	0.0338	0.0123	0.0166
C(6)	0.0371	0.0432	0.0462	0.0239	0.0146	0.0074
C(7)	0.0213	0.0434	0.0353	0.0188	0.0071	0.0041
C(8)	0.0096	0.0204	0.0381	0.0019	-0.0006	-0.0028
C(9)	0.0064	0.0248	0.0141	0.0052	-0.0005	0.0073
C(10)	0.0262	0.0308	0.0277	0.0093	0.0082	0.0065
C(11)	0.0246	0.0356	0.0165	0.0105	0.0101	0.0083
C(12)	0.0242	0.0386	0.0316	0.0210	0.0154	0.0186
C(13)	0.0363	0.0324	0.0308	0.0189	0.0157	-0.0009
C(14)	0.0238	0.0182	0.0310	0.0086	0.0155	0.0030
C(15)	0.0144	0.0224	0.0188	0.0063	0.0057	0.0085
C(16)	0.0179	0.0264	0.0255	0.0076	0.0055	0.0049
C(17)	0.0294	0.0210	0.0303	0.0133	0.0153	0.0125
C(18)	0.0239	0.0207	0.0381	-0.0091	0.0154	0.0015
C(19)	0.0168	0.0312	0.0278	0.0134	-0.0022	0.0049
C(20)	0.0240	0.0279	0.0280	0.0134	0.0137	0.0040
C(21)	0.0126	0.0168	0.0249	0.0087	0.0044	0.0057
C(22)	0.0228	0.0271	0.0332	0.0176	0.0143	0.0089
C(23)	0.0336	0.0340	0.0337	0.0141	0.0117	0.0140
C(24)	0.0378	0.0339	0.0579	0.0212	0.0329	0.0268
C(25)	0.0469	0.0335	0.0565	0.0187	0.0369	0.0114
C(26)	0.0224	0.0247	0.0405	0.0020	0.0165	-0.0007
C(27)	0.0266	0.0203	0.0396	0.0078	0.0195	0.0055
C(28)	0.0233	0.0178	0.0330	0.0119	0.0176	0.0095
C(29)	0.0362	0.0363	0.0262	0.0205	0.0115	0.0086
C(30)	0.0507	0.0398	0.0446	0.0216	0.0370	0.0143
C(31)	0.0543	0.0529	0.0254	0.0334	0.0209	0.0179
C(32)	0.0417	0.0434	0.0220	0.0190	0.0079	0.0058
C(33)	0.0320	0.0235	0.0296	0.0098	0.0141	0.0130
C(34)	0.0168	0.0335	0.0286	0.0162	0.0103	0.0103
C(35)	0.0153	0.0273	0.0239	0.0074	0.0061	0.0081
C(36)	0.0244	0.0351	0.0284	0.0129	0.0061	0.0040
C(37)	0.0314	0.0452	0.0285	0.0139	0.0088	-0.0079
C(38)	0.0378	0.0518	0.0193	0.0172	0.0083	-0.0045
C(39)	0.0286	0.0579	0.0173	0.0237	0.0008	0.0031
C(40)	0.0197	0.0256	0.0324	0.0042	0.0146	0.0006
C(41)	0.0220	0.0127	0.0228	0.0051	0.0027	-0.0047
C(42)	0.0273	0.0235	0.0257	0.0175	0.0089	0.0059
C(43)	0.0236	0.0319	0.0300	0.0072	0.0105	0.0020
C(44)	0.0278	0.0246	0.0335	0.0024	0.0147	0.0096
C(45)	0.0351	0.0359	0.0337	0.0205	0.0118	0.0160
C(46)	0.0208	0.0264	0.0233	0.0123	0.0058	0.0067
C(47)	0.0280	0.0179	0.0368	0.0112	0.0280	0.0125

atom	U11	U22	U33	U12	U13	U23
C(48)	0.0193	0.0144	0.0257	0.0063	0.0161	0.0082
C(49)	0.0233	0.0413	0.0247	0.0147	0.0058	0.0095
C(50)	0.0281	0.0291	0.0455	0.0160	0.0238	0.0100
C(51)	0.0262	0.0224	0.0407	0.0151	0.0157	0.0138
C(52)	0.0212	0.0235	0.0239	0.0098	0.0028	0.0136
C(53)	0.011(5)	0.023(5)	0.027(6)	0.003(4)	0.001(4)	-0.003(4)
C(54)	0.120(13)	0.057(10)	0.203(18)	0.016(10)	0.128(13)	0.016(11
C(55)	0.054(8)	0.087(10)	0.034(7)	0.050(8)	0.036(6)	0.039(7)
C(56)	0.117(14)	0.092(13)	0.091(13)	0.096(12)	0.003(10)	0.034(10
C(57)	0.095(11)	0.063(10)	0.068(10)	0.013(8)	0.041(8)	-0.003(8)
B(1)	0.012(5)	0.024(6)	0.019(6)	0.006(5)	0.007(4)	0.002(5)

Table 5. Positional parameters and B(eq) for **3**.

atom	x	y	z	B(eq)
Ir(01)	0.56041(2)	0.24978(2)	0.728235(9)	1.457(8)
P(1)	0.4344(1)	0.1889(1)	0.64646(7)	1.55(6)
P(2)	0.7270(1)	0.2442(1)	0.68448(6)	1.48(5)
P(3)	0.6167(1)	0.1276(1)	0.76630(7)	1.51(6)
C(1)	0.4263(5)	0.2933(4)	0.7800(3)	2.4(3)
C(2)	0.4104(5)	0.3320(4)	0.7266(3)	2.3(3)
C(3)	0.5046(5)	0.3746(4)	0.7103(3)	2.1(3)
C(4)	0.5249(5)	0.1304(4)	0.6067(3)	1.7(2)
C(5)	0.7603(5)	0.1462(4)	0.6606(3)	1.5(2)
C(6)	0.6082(5)	0.0534(4)	0.7110(3)	1.5(2)
C(7)	0.3175(5)	0.1201(4)	0.6602(3)	1.8(3)
C(8)	0.2906(5)	0.1154(4)	0.7147(3)	2.2(3)
C(9)	0.2031(6)	0.0624(5)	0.7266(3)	3.1(3)
C(10)	0.1411(6)	0.0152(4)	0.6827(4)	3.2(3)
C(11)	0.1672(5)	0.0190(4)	0.6277(3)	2.6(3)
C(12)	0.2541(5)	0.0710(4)	0.6161(3)	2.3(3)
C(13)	0.3428(5)	0.2576(4)	0.5936(2)	1.7(2)
C(14)	0.2158(5)	0.2632(4)	0.5869(3)	2.1(3)
C(15)	0.1525(5)	0.3172(4)	0.5479(3)	2.5(3)
C(16)	0.2119(6)	0.3636(4)	0.5148(3)	3.0(3)
C(17)	0.3368(6)	0.3581(4)	0.5221(3)	2.8(3)
C(18)	0.4000(5)	0.3064(4)	0.5610(3)	2.6(3)
C(19)	0.7230(5)	0.3096(4)	0.6226(3)	1.6(2)
C(20)	0.7135(6)	0.3916(4)	0.6314(3)	2.2(3)
C(21)	0.7098(6)	0.4435(4)	0.5869(3)	2.7(3)
C(22)	0.7125(7)	0.4187(4)	0.5320(3)	3.1(3)
C(23)	0.7243(6)	0.3385(4)	0.5221(3)	2.6(3)
C(24)	0.7295(5)	0.2849(4)	0.5666(3)	2.1(2)
C(25)	0.8736(5)	0.2787(4)	0.7269(3)	1.7(2)
C(26)	0.8824(5)	0.3295(4)	0.7746(3)	1.8(2)
C(27)	0.9969(5)	0.3588(4)	0.8016(3)	2.2(3)
C(28)	1.1001(5)	0.3378(4)	0.7821(3)	2.5(3)
C(29)	1.0909(5)	0.2866(5)	0.7357(3)	3.0(3)
C(30)	0.9784(5)	0.2585(4)	0.7085(3)	2.4(3)
C(31)	0.7741(5)	0.1255(4)	0.8096(3)	1.8(2)
C(32)	0.8613(5)	0.0711(4)	0.7986(3)	1.8(3)
C(33)	0.9784(5)	0.0725(4)	0.8312(3)	2.2(3)
C(34)	1.0118(5)	0.1271(4)	0.8749(3)	2.6(3)
C(35)	0.9264(6)	0.1803(4)	0.8870(3)	2.6(3)
C(36)	0.8088(5)	0.1795(4)	0.8543(3)	1.8(2)
C(37)	0.5340(5)	0.0865(4)	0.8196(3)	1.9(3)
C(38)	0.5038(6)	0.0078(4)	0.8190(3)	2.5(3)
C(39)	0.4432(7)	-0.0237(5)	0.8594(3)	3.6(4)
C(40)	0.4081(7)	0.0251(4)	0.9007(3)	3.4(3)
C(41)	0.4405(6)	0.1045(4)	0.9026(3)	2.8(3)
C(42)	0.5011(5)	0.1357(4)	0.8616(3)	2.2(3)
C(43)	0.6762(5)	0.0052(4)	0.6159(3)	1.4(2)
C(44)	0.5915(5)	-0.0379(4)	0.5768(3)	1.9(3)
C(45)	0.6228(6)	-0.1077(4)	0.5512(3)	2.1(3)
C(46)	0.7423(6)	-0.1340(4)	0.5641(3)	2.5(3)

atom	x	y	z	B(eq)
C(47)	0.8277(5)	-0.0923(4)	0.6031(3)	2.5(3)
C(48)	0.7937(5)	-0.0239(4)	0.6276(3)	2.0(3)
C(49)	0.8086(6)	0.1932(4)	0.4249(3)	2.9(3)
C(50)	0.9276(6)	0.1876(4)	0.4524(3)	2.5(3)
C(51)	0.9628(6)	0.1358(4)	0.4973(3)	2.9(3)
C(52)	0.8784(7)	0.0903(4)	0.5168(3)	3.1(3)
C(53)	0.7574(7)	0.0957(4)	0.4895(3)	3.4(4)
C(54)	0.7222(6)	0.1458(5)	0.4442(3)	3.2(3)
B(1)	0.6409(6)	0.0852(4)	0.6479(3)	1.6(1)

Table 6. Intramolecular Distances Involving the Nonhydrogen Atoms for **3**.

atom	atom	distance	atom	atom	distance
Ir(01)	P(1)	2.388(2)	C(13)	C(14)	1.406(7)
Ir(01)	P(2)	2.320(1)	C(13)	C(18)	1.382(9)
Ir(01)	P(3)	2.307(2)	C(14)	C(15)	1.391(8)
Ir(01)	C(1)	2.255(6)	C(15)	C(16)	1.38(1)
Ir(01)	C(2)	2.186(6)	C(16)	C(17)	1.381(9)
Ir(01)	C(3)	2.234(6)	C(17)	C(18)	1.364(9)
P(1)	C(4)	1.820(6)	C(19)	C(20)	1.421(9)
P(1)	C(7)	1.840(6)	C(19)	C(24)	1.408(9)
P(1)	C(13)	1.862(6)	C(20)	C(21)	1.370(9)
P(2)	C(5)	1.826(6)	C(21)	C(22)	1.37(1)
P(2)	C(19)	1.835(6)	C(22)	C(23)	1.40(1)
P(2)	C(25)	1.841(6)	C(23)	C(24)	1.388(9)
P(3)	C(6)	1.808(6)	C(25)	C(26)	1.411(9)
P(3)	C(31)	1.854(6)	C(25)	C(30)	1.379(8)
P(3)	C(37)	1.853(6)	C(26)	C(27)	1.405(8)
C(1)	C(2)	1.405(9)	C(27)	C(28)	1.381(9)
C(2)	C(3)	1.402(9)	C(28)	C(29)	1.39(1)
C(4)	B(1)	1.651(9)	C(29)	C(30)	1.381(9)
C(5)	B(1)	1.675(9)	C(31)	C(32)	1.410(8)
C(6)	B(1)	1.699(9)	C(31)	C(36)	1.396(8)
C(7)	C(8)	1.389(9)	C(32)	C(33)	1.383(8)
C(7)	C(12)	1.411(9)	C(33)	C(34)	1.386(9)
C(8)	C(9)	1.405(9)	C(34)	C(35)	1.391(9)
C(9)	C(10)	1.38(1)	C(35)	C(36)	1.388(8)
C(10)	C(11)	1.39(1)	C(37)	C(38)	1.384(9)
C(11)	C(12)	1.388(9)	C(37)	C(42)	1.407(9)
C(38)	C(39)	1.39(1)	C(39)	C(40)	1.40(1)
C(40)	C(41)	1.40(1)	C(41)	C(42)	1.400(9)
C(43)	C(44)	1.394(8)	C(43)	C(48)	1.384(8)
C(43)	B(1)	1.648(9)	C(44)	C(45)	1.412(8)
C(45)	C(46)	1.388(9)	C(46)	C(47)	1.384(9)
C(47)	C(48)	1.390(9)	C(49)	C(50)	1.365(9)
C(49)	C(54)	1.41(1)	C(50)	C(51)	1.38(1)
C(51)	C(52)	1.38(1)	C(52)	C(53)	1.38(1)
C(53)	C(54)	1.37(1)			

Distances are in angstroms. Estimated standard deviations in the least significant figure are given in parentheses.

Table 7. Intramolecular Bond Angles Involving the Nonhydrogen Atoms for **3**.

atom	atom	atom	angle	atom	atom	atom	angle
P(1)	Ir(01)	P(2)	91.05(5)	C(19)	P(2)	C(25)	96.6(3)
P(1)	Ir(01)	P(3)	89.69(6)	Ir(01)	P(3)	C(6)	112.3(2)
P(1)	Ir(01)	C(1)	103.5(2)	Ir(01)	P(3)	C(31)	112.9(2)
P(1)	Ir(01)	C(2)	86.4(2)	Ir(01)	P(3)	C(37)	118.2(2)
P(1)	Ir(01)	C(3)	99.4(2)	C(6)	P(3)	C(31)	106.8(3)
P(2)	Ir(01)	P(3)	87.47(6)	C(6)	P(3)	C(37)	105.6(3)
P(2)	Ir(01)	C(1)	161.3(2)	C(31)	P(3)	C(37)	99.8(3)
P(2)	Ir(01)	C(2)	135.1(2)	Ir(01)	C(1)	C(2)	68.9(3)
P(2)	Ir(01)	C(3)	100.1(2)	Ir(01)	C(2)	C(1)	74.2(3)
P(3)	Ir(01)	C(1)	104.2(2)	Ir(01)	C(2)	C(3)	73.4(3)
P(3)	Ir(01)	C(2)	137.3(2)	C(1)	C(2)	C(3)	121.9(6)
P(3)	Ir(01)	C(3)	168.1(2)	Ir(01)	C(3)	C(2)	69.6(4)
C(1)	Ir(01)	C(2)	36.8(2)	P(1)	C(4)	B(1)	114.0(4)
C(1)	Ir(01)	C(3)	66.3(2)	P(2)	C(5)	B(1)	114.5(4)
C(2)	Ir(01)	C(3)	37.0(2)	P(3)	C(6)	B(1)	115.1(4)
Ir(01)	P(1)	C(4)	110.9(2)	P(1)	C(7)	C(8)	120.0(5)
Ir(01)	P(1)	C(7)	117.4(2)	P(1)	C(7)	C(12)	121.2(5)
Ir(01)	P(1)	C(13)	115.2(2)	C(8)	C(7)	C(12)	118.8(6)
C(4)	P(1)	C(7)	103.7(3)	C(7)	C(8)	C(9)	121.2(6)
C(4)	P(1)	C(13)	106.7(3)	C(8)	C(9)	C(10)	119.3(7)
C(7)	P(1)	C(13)	101.7(3)	C(9)	C(10)	C(11)	120.3(6)
Ir(01)	P(2)	C(5)	114.3(2)	C(10)	C(11)	C(12)	120.4(6)
Ir(01)	P(2)	C(19)	116.2(2)	C(7)	C(12)	C(11)	120.1(6)
Ir(01)	P(2)	C(25)	117.2(2)	P(1)	C(13)	C(14)	121.9(5)
C(5)	P(2)	C(19)	106.4(3)	P(1)	C(13)	C(18)	119.9(4)
C(5)	P(2)	C(25)	104.1(3)	C(14)	C(13)	C(18)	118.2(6)
C(13)	C(14)	C(15)	119.3(6)	C(33)	C(34)	C(35)	119.9(6)
C(14)	C(15)	C(16)	121.1(6)	C(34)	C(35)	C(36)	119.8(6)
C(15)	C(16)	C(17)	119.1(6)	C(31)	C(36)	C(35)	121.0(6)
C(16)	C(17)	C(18)	120.2(7)	P(3)	C(37)	C(38)	121.1(5)
C(13)	C(18)	C(17)	122.1(6)	P(3)	C(37)	C(42)	119.8(5)
P(2)	C(19)	C(20)	118.2(5)	C(38)	C(37)	C(42)	119.1(6)
P(2)	C(19)	C(24)	125.0(5)	C(37)	C(38)	C(39)	121.4(7)
C(20)	C(19)	C(24)	116.8(6)	C(38)	C(39)	C(40)	119.9(7)
C(19)	C(20)	C(21)	121.0(6)	C(39)	C(40)	C(41)	119.2(6)
C(20)	C(21)	C(22)	121.9(7)	C(40)	C(41)	C(42)	120.4(6)
C(21)	C(22)	C(23)	118.7(7)	C(37)	C(42)	C(41)	119.9(6)
C(22)	C(23)	C(24)	120.5(7)	C(44)	C(43)	C(48)	115.9(6)
C(19)	C(24)	C(23)	121.2(6)	C(44)	C(43)	B(1)	123.1(5)
P(2)	C(25)	C(26)	122.8(4)	C(48)	C(43)	B(1)	120.9(5)
P(2)	C(25)	C(30)	118.3(5)	C(43)	C(44)	C(45)	122.2(5)
C(26)	C(25)	C(30)	118.8(5)	C(44)	C(45)	C(46)	119.5(6)
C(25)	C(26)	C(27)	119.3(6)	C(45)	C(46)	C(47)	119.2(6)
C(26)	C(27)	C(28)	120.6(6)	C(46)	C(47)	C(48)	119.8(6)
C(27)	C(28)	C(29)	119.7(6)	C(43)	C(48)	C(47)	123.3(6)
C(28)	C(29)	C(30)	119.9(6)	C(50)	C(49)	C(54)	118.4(7)
C(25)	C(30)	C(29)	121.6(6)	C(49)	C(50)	C(51)	120.8(6)
P(3)	C(31)	C(32)	122.1(5)	C(50)	C(51)	C(52)	120.8(6)
P(3)	C(31)	C(36)	119.5(4)	C(51)	C(52)	C(53)	119.0(7)
C(32)	C(31)	C(36)	118.5(5)	C(52)	C(53)	C(54)	120.4(7)
C(31)	C(32)	C(33)	120.2(6)	C(49)	C(54)	C(53)	120.4(6)
C(32)	C(33)	C(34)	120.6(6)	C(4)	B(1)	C(5)	108.8(5)

atom	atom	atom	angle	atom	atom	atom	angle
C(4)	B(1)	C(6)	112.5(5)	C(4)	B(1)	C(43)	110.4(5)
C(5)	B(1)	C(6)	110.6(5)	C(5)	B(1)	C(43)	109.6(5)
C(6)	B(1)	C(43)	104.8(5)				

Angles are in degrees. Estimated standard deviations in the least significant figure are given in parentheses.

Table 8. Anisotropic Displacement Parameters for **3**.

atom	U11	U22	U33	U12	U13	U23
Ir(01)	0.0210(1)	0.0173(1)	0.0179(1)	0.0002(2)	0.00614(7)	-0.0010(2)
P(1)	0.0209(7)	0.0193(9)	0.0187(9)	0.0003(7)	0.0039(7)	0.0011(8)
P(2)	0.0205(6)	0.0188(8)	0.0172(7)	-0.003(1)	0.0046(5)	0.001(1)
P(3)	0.0231(7)	0.020(1)	0.0157(9)	-0.0002(7)	0.0069(7)	-0.0013(7)
C(1)	0.030(3)	0.033(4)	0.033(4)	0.013(3)	0.022(3)	0.004(4)
C(2)	0.026(3)	0.031(4)	0.029(4)	0.008(3)	0.002(3)	-0.003(4)
C(3)	0.027(3)	0.016(4)	0.038(4)	0.003(3)	0.005(3)	0.001(3)
C(4)	0.029(3)	0.017(3)	0.018(4)	-0.003(3)	0.004(3)	-0.008(3)
C(5)	0.025(3)	0.017(3)	0.017(4)	0.001(3)	0.008(3)	0.002(3)
C(6)	0.022(3)	0.019(3)	0.015(3)	-0.001(3)	0.003(3)	-0.005(3)
C(7)	0.020(3)	0.021(4)	0.026(4)	-0.002(3)	0.003(3)	0.000(3)
C(8)	0.028(3)	0.030(4)	0.025(4)	-0.007(3)	0.005(3)	-0.005(3)
C(9)	0.035(4)	0.048(5)	0.043(5)	-0.010(4)	0.022(4)	0.001(4)
C(10)	0.027(4)	0.029(4)	0.070(6)	-0.006(3)	0.015(4)	0.013(4)
C(11)	0.024(3)	0.028(4)	0.044(5)	-0.007(3)	0.000(3)	-0.010(4)
C(12)	0.033(3)	0.028(4)	0.029(4)	0.002(3)	0.013(3)	0.003(3)
C(13)	0.028(3)	0.017(4)	0.017(3)	0.006(4)	0.000(2)	-0.008(4)
C(14)	0.030(3)	0.016(5)	0.030(4)	-0.000(3)	-0.002(3)	0.001(3)
C(15)	0.030(3)	0.028(4)	0.035(4)	0.009(3)	-0.003(3)	-0.002(4)
C(16)	0.046(4)	0.031(4)	0.031(5)	0.015(4)	-0.004(3)	-0.001(4)
C(17)	0.045(4)	0.029(4)	0.033(5)	0.001(3)	0.005(3)	0.005(4)
C(18)	0.030(3)	0.029(4)	0.039(5)	0.001(3)	0.008(3)	-0.002(4)
C(19)	0.024(3)	0.020(4)	0.018(4)	-0.004(3)	0.005(3)	0.002(3)
C(20)	0.035(4)	0.033(4)	0.017(4)	0.002(3)	0.005(3)	0.001(3)
C(21)	0.052(4)	0.017(4)	0.038(5)	-0.004(3)	0.016(4)	0.002(3)
C(22)	0.070(5)	0.031(4)	0.025(5)	0.000(4)	0.022(4)	0.005(4)
C(23)	0.038(4)	0.037(5)	0.025(4)	0.005(3)	0.009(3)	-0.004(4)
C(24)	0.032(3)	0.025(3)	0.022(4)	-0.005(3)	0.006(3)	-0.000(3)
C(25)	0.019(3)	0.024(4)	0.020(4)	-0.006(2)	0.001(3)	-0.001(3)
C(26)	0.023(3)	0.021(4)	0.025(4)	-0.001(3)	0.003(3)	0.000(3)
C(27)	0.032(3)	0.027(4)	0.022(4)	0.001(3)	0.003(3)	0.001(3)
C(28)	0.026(3)	0.035(4)	0.029(4)	-0.001(3)	-0.002(3)	-0.001(4)
C(29)	0.023(3)	0.041(4)	0.047(5)	-0.001(3)	0.004(3)	-0.008(4)
C(30)	0.031(3)	0.031(4)	0.034(4)	-0.004(4)	0.016(3)	-0.016(4)
C(31)	0.028(3)	0.019(4)	0.021(4)	-0.006(3)	0.009(3)	0.004(3)
C(32)	0.033(3)	0.020(4)	0.019(4)	-0.001(3)	0.011(3)	0.004(3)

Table 9. Positional parameters and B(eq) for **4**.

atom	x	y	z	B(eq)
Ir(01)	0.91959(3)	0.23248(1)	0.82731(2)	1.62(1)
Cl(1)	0.3239(5)	0.0871(2)	0.6644(3)	9.6(3)
Cl(2)	0.1553(4)	-0.0032(2)	0.6717(2)	9.9(2)
Cl(3)	0.433(2)	0.050(1)	0.691(1)	9.5
P(1)	1.1270(2)	0.23225(8)	0.85563(9)	1.78(7)
P(2)	0.9021(2)	0.25810(8)	0.9463(1)	1.91(7)
P(3)	0.9293(2)	0.33107(8)	0.7957(1)	1.77(7)
P(4)	0.8751(2)	0.17966(8)	0.7195(1)	2.22(8)
C(1)	0.9110(6)	0.1586(3)	0.8951(4)	2.0(3)
C(2)	0.9168(7)	0.0968(3)	0.8895(4)	2.3(3)
C(3)	0.9162(7)	0.0620(3)	0.9500(5)	2.9(4)
C(4)	0.9106(7)	0.0862(3)	1.0191(4)	2.8(3)
C(5)	0.9031(7)	0.1461(3)	1.0266(4)	2.7(3)
C(6)	0.9038(7)	0.1810(3)	0.9648(4)	2.1(3)
C(7)	0.7614(7)	0.2856(3)	0.9642(4)	2.5(3)
C(8)	0.6653(8)	0.2483(3)	0.9573(4)	3.0(4)
C(9)	0.5571(8)	0.2668(5)	0.9736(5)	4.4(5)
C(10)	0.5448(9)	0.3233(5)	0.9964(5)	4.9(5)
C(11)	0.637(1)	0.3616(4)	1.0015(5)	4.8(5)
C(12)	0.7464(8)	0.3437(4)	0.9864(5)	3.7(4)
C(13)	1.0160(7)	0.3014(3)	0.9982(4)	2.2(3)
C(14)	1.1826(6)	0.1654(3)	0.9048(4)	2.2(3)
C(15)	1.1914(7)	0.1599(3)	0.9807(4)	2.4(3)
C(16)	1.2209(8)	0.1065(4)	1.0139(5)	3.4(4)
C(17)	1.2419(8)	0.0581(4)	0.9718(6)	3.9(4)
C(18)	1.2337(8)	0.0632(3)	0.8982(5)	3.8(4)
C(19)	1.2044(7)	0.1159(3)	0.8643(4)	2.9(4)
C(20)	1.2227(6)	0.2327(3)	0.7847(4)	1.9(3)
C(21)	1.3428(6)	0.2301(4)	0.8054(4)	2.8(3)
C(22)	1.4175(7)	0.2313(4)	0.7542(4)	3.4(4)
C(23)	1.3732(8)	0.2344(4)	0.6808(5)	3.7(4)
C(24)	1.2552(8)	0.2383(4)	0.6583(4)	3.2(4)
C(25)	1.1785(6)	0.2376(3)	0.7110(4)	2.3(3)
C(26)	1.1845(7)	0.2947(3)	0.9130(4)	1.8(3)
C(27)	1.0147(7)	0.3561(3)	0.7244(4)	2.2(3)
C(28)	1.1298(8)	0.3750(3)	0.7420(4)	3.0(4)
C(29)	1.1946(8)	0.3910(4)	0.6868(5)	3.7(4)
C(30)	1.1420(9)	0.3877(4)	0.6139(5)	4.2(5)
C(31)	1.0281(9)	0.3690(4)	0.5969(4)	3.9(4)
C(32)	0.9654(8)	0.3525(3)	0.6517(4)	3.1(4)
C(33)	0.7917(7)	0.3700(3)	0.7659(4)	2.1(3)
C(34)	0.6838(8)	0.3440(4)	0.7604(6)	4.3(5)
C(35)	0.5808(8)	0.3755(4)	0.7396(7)	6.0(6)
C(36)	0.5859(8)	0.4339(4)	0.7248(5)	4.4(5)
C(37)	0.6924(9)	0.4603(3)	0.7300(5)	4.2(4)
C(38)	0.7926(8)	0.4295(3)	0.7505(5)	3.5(4)
C(39)	0.9933(7)	0.3716(3)	0.8772(4)	2.0(3)
C(40)	1.1568(7)	0.3935(3)	0.9895(4)	2.2(3)
C(41)	1.0977(8)	0.4310(3)	1.0327(4)	3.2(4)
C(42)	1.1526(8)	0.4785(3)	1.0696(5)	3.6(4)

atom	x	y	z	B(eq)
C(43)	1.265(1)	0.4926(3)	1.0652(5)	4.2(4)
C(44)	1.3271(8)	0.4573(3)	1.0232(5)	3.4(4)
C(45)	1.2724(8)	0.4094(3)	0.9861(4)	2.8(4)
C(46)	0.8362(7)	0.2175(3)	0.6330(4)	2.7(3)
C(47)	0.9740(7)	0.1231(3)	0.6960(4)	2.6(3)
C(48)	0.7415(8)	0.1377(3)	0.7211(5)	3.5(4)
C(49)	0.299(1)	0.0145(6)	0.6546(8)	5.8(3)
C(50)	0.502(1)	0.0552(7)	0.7881(9)	5.9(3)
C(51)	0.478(1)	0.0088(5)	0.8341(6)	2.7(2)
C(52)	0.595(2)	0.0117(7)	0.863(1)	6.1(4)
C(53)	0.513(2)	0.0040(7)	0.876(1)	6.0(4)
C(54)	0.547(3)	0.044(1)	0.949(2)	7.1(8)
C(55)	0.594(2)	0.083(1)	0.921(1)	11.1(6)
C(56)	0.625(1)	0.1002(5)	0.9036(6)	4.5(2)
C(57)	0.522(1)	0.1268(6)	0.8721(8)	4.3(3)
C(58)	0.513(3)	0.089(2)	0.841(2)	14(1)
B(1)	1.0887(7)	0.3397(3)	0.9435(4)	1.7(1)

Table 10. Intramolecular Distances Involving the Nonhydrogen Atoms for **4**.

atom	atom	distance	atom	atom	distance
Ir(01)	P(1)	2.377(2)	C(4)	C(5)	1.38(1)
Ir(01)	P(2)	2.320(2)	C(5)	C(6)	1.40(1)
Ir(01)	P(3)	2.337(2)	C(7)	C(8)	1.39(1)
Ir(01)	P(4)	2.325(2)	C(7)	C(12)	1.41(1)
Ir(01)	C(1)	2.116(7)	C(8)	C(9)	1.40(1)
Cl(1)	Cl(3)	1.53(3)	C(9)	C(10)	1.37(1)
Cl(1)	C(49)	1.69(1)	C(10)	C(11)	1.37(1)
Cl(2)	C(49)	1.78(2)	C(11)	C(12)	1.40(1)
Cl(3)	C(49)	1.79(3)	C(13)	B(1)	1.66(1)
Cl(3)	C(50)	1.87(3)	C(14)	C(15)	1.40(1)
P(1)	C(14)	1.845(7)	C(14)	C(19)	1.40(1)
P(1)	C(20)	1.842(7)	C(15)	C(16)	1.39(1)
P(1)	C(26)	1.844(7)	C(16)	C(17)	1.40(1)
P(2)	C(6)	1.796(7)	C(17)	C(18)	1.36(1)
P(2)	C(7)	1.821(8)	C(18)	C(19)	1.38(1)
P(2)	C(13)	1.804(8)	C(20)	C(21)	1.38(1)
P(3)	C(27)	1.855(7)	C(20)	C(25)	1.39(1)
P(3)	C(33)	1.834(8)	C(21)	C(22)	1.38(1)
P(3)	C(39)	1.831(7)	C(22)	C(23)	1.38(1)
P(4)	C(46)	1.817(8)	C(23)	C(24)	1.37(1)
P(4)	C(47)	1.823(8)	C(24)	C(25)	1.42(1)
P(4)	C(48)	1.823(8)	C(26)	B(1)	1.67(1)
C(1)	C(2)	1.420(9)	C(27)	C(28)	1.39(1)
C(1)	C(6)	1.40(1)	C(27)	C(32)	1.38(1)
C(2)	C(3)	1.38(1)	C(28)	C(29)	1.41(1)
C(3)	C(4)	1.41(1)	C(29)	C(30)	1.39(1)
C(30)	C(31)	1.38(1)	C(56)	C(57)	1.39(2)
C(31)	C(32)	1.39(1)	C(56)	C(58)	1.62(4)
C(33)	C(34)	1.37(1)	C(57)	C(58)	1.03(3)
C(33)	C(38)	1.39(1)	C(34)	C(35)	1.40(1)
C(35)	C(36)	1.37(1)	C(36)	C(37)	1.36(1)
C(37)	C(38)	1.36(1)	C(39)	B(1)	1.69(1)
C(40)	C(41)	1.42(1)	C(40)	C(45)	1.40(1)
C(40)	B(1)	1.63(1)	C(41)	C(42)	1.39(1)
C(42)	C(43)	1.36(1)	C(43)	C(44)	1.39(1)
C(44)	C(45)	1.39(1)	C(50)	C(51)	1.41(2)
C(50)	C(58)	1.24(3)	C(51)	C(52)	1.38(2)
C(51)	C(53)	0.83(2)	C(52)	C(53)	1.04(2)
C(53)	C(54)	1.62(4)	C(54)	C(55)	1.21(3)
C(55)	C(56)	0.66(2)	C(55)	C(57)	1.52(2)
C(55)	C(58)	1.63(4)			

Distances are in angstroms. Estimated standard deviations in the least significant figure are given in parentheses.

Table 11. Intramolecular Bond Angles Involving the Nonhydrogen Atoms for **4**.

atom	atom	atom	angle	atom	atom	atom	angle
P(1)	Ir(01)	P(2)	91.22(6)	Ir(01)	P(3)	C(27)	121.8(2)
P(1)	Ir(01)	P(3)	88.41(7)	Ir(01)	P(3)	C(33)	118.1(2)
P(1)	Ir(01)	P(4)	105.84(7)	Ir(01)	P(3)	C(39)	108.1(2)
P(1)	Ir(01)	C(1)	90.2(2)	C(27)	P(3)	C(33)	99.7(3)
P(2)	Ir(01)	P(3)	90.51(6)	C(27)	P(3)	C(39)	103.8(3)
P(2)	Ir(01)	P(4)	155.28(7)	C(33)	P(3)	C(39)	103.1(3)
P(2)	Ir(01)	C(1)	67.6(2)	Ir(01)	P(4)	C(46)	120.2(2)
P(3)	Ir(01)	P(4)	107.39(7)	Ir(01)	P(4)	C(47)	120.6(3)
P(3)	Ir(01)	C(1)	158.1(2)	Ir(01)	P(4)	C(48)	109.7(3)
P(4)	Ir(01)	C(1)	94.0(2)	C(46)	P(4)	C(47)	102.0(4)
Cl(3)	Cl(1)	C(49)	67(1)	C(46)	P(4)	C(48)	99.7(4)
Cl(1)	Cl(3)	C(49)	61(1)	C(47)	P(4)	C(48)	101.2(4)
Cl(1)	Cl(3)	C(50)	119(2)	Ir(01)	C(1)	C(2)	138.1(5)
C(49)	Cl(3)	C(50)	128(2)	Ir(01)	C(1)	C(6)	105.6(5)
Ir(01)	P(1)	C(14)	112.0(2)	C(2)	C(1)	C(6)	116.1(6)
Ir(01)	P(1)	C(20)	122.6(2)	C(1)	C(2)	C(3)	120.7(7)
Ir(01)	P(1)	C(26)	112.9(2)	C(2)	C(3)	C(4)	121.4(6)
C(14)	P(1)	C(20)	98.9(3)	C(3)	C(4)	C(5)	119.7(7)
C(14)	P(1)	C(26)	106.9(3)	C(4)	C(5)	C(6)	118.4(7)
C(20)	P(1)	C(26)	101.7(3)	P(2)	C(6)	C(1)	100.5(5)
Ir(01)	P(2)	C(6)	86.2(2)	P(2)	C(6)	C(5)	135.8(6)
Ir(01)	P(2)	C(7)	118.0(2)	C(1)	C(6)	C(5)	123.7(6)
Ir(01)	P(2)	C(13)	118.9(2)	P(2)	C(7)	C(8)	119.7(6)
C(6)	P(2)	C(7)	106.8(3)	P(2)	C(7)	C(12)	122.0(7)
C(6)	P(2)	C(13)	116.8(3)	C(8)	C(7)	C(12)	118.3(7)
C(7)	P(2)	C(13)	108.3(3)	C(7)	C(8)	C(9)	121.6(8)
C(8)	C(9)	C(10)	119.3(9)	C(28)	C(29)	C(30)	119.2(8)
C(9)	C(10)	C(11)	120.5(8)	C(29)	C(30)	C(31)	120.0(8)
C(10)	C(11)	C(12)	121.1(9)	C(30)	C(31)	C(32)	120.4(8)
C(7)	C(12)	C(11)	119.2(9)	C(27)	C(32)	C(31)	120.8(8)
P(2)	C(13)	B(1)	111.1(5)	P(3)	C(33)	C(34)	123.4(6)
P(1)	C(14)	C(15)	122.5(6)	P(3)	C(33)	C(38)	120.2(6)
P(1)	C(14)	C(19)	118.8(6)	C(34)	C(33)	C(38)	116.4(7)
C(15)	C(14)	C(19)	118.3(7)	C(33)	C(34)	C(35)	121.6(8)
C(14)	C(15)	C(16)	119.9(7)	C(34)	C(35)	C(36)	120.0(9)
C(15)	C(16)	C(17)	120.2(8)	C(35)	C(36)	C(37)	119.0(8)
C(16)	C(17)	C(18)	120.2(8)	C(36)	C(37)	C(38)	120.9(8)
C(17)	C(18)	C(19)	120.4(8)	C(33)	C(38)	C(37)	122.1(8)
C(14)	C(19)	C(18)	121.0(8)	P(3)	C(39)	B(1)	121.2(5)
P(1)	C(20)	C(21)	119.3(5)	C(41)	C(40)	C(45)	114.5(7)
P(1)	C(20)	C(25)	122.0(5)	C(41)	C(40)	B(1)	121.1(7)
C(21)	C(20)	C(25)	118.7(6)	C(45)	C(40)	B(1)	124.3(7)
C(20)	C(21)	C(22)	121.1(7)	C(40)	C(41)	C(42)	122.0(8)
C(21)	C(22)	C(23)	120.1(8)	C(41)	C(42)	C(43)	121.9(8)
C(22)	C(23)	C(24)	120.5(7)	C(42)	C(43)	C(44)	118.4(8)
C(23)	C(24)	C(25)	119.3(7)	C(43)	C(44)	C(45)	119.9(8)
C(20)	C(25)	C(24)	120.2(7)	C(40)	C(45)	C(44)	123.3(8)
P(1)	C(26)	B(1)	118.2(5)	Cl(1)	C(49)	Cl(2)	110.6(9)
P(3)	C(27)	C(28)	121.6(6)	Cl(1)	C(49)	Cl(3)	52.3(9)
P(3)	C(27)	C(32)	119.3(6)	Cl(2)	C(49)	Cl(3)	145(1)
C(28)	C(27)	C(32)	119.0(7)	Cl(3)	C(50)	C(51)	116(1)
C(27)	C(28)	C(29)	120.5(8)	Cl(3)	C(50)	C(58)	142(2)

C(51)	C(50)	C(58)	90(2)	C(56)	C(58)	C(57)	58(2)
C(50)	C(51)	C(52)	86(1)	C(13)	B(1)	C(26)	107.8(5)
C(50)	C(51)	C(53)	124(2)	C(13)	B(1)	C(39)	109.7(6)
C(52)	C(51)	C(53)	48(2)	C(13)	B(1)	C(40)	109.1(6)
C(51)	C(52)	C(53)	37(1)	C(26)	B(1)	C(39)	114.5(6)
C(51)	C(53)	C(52)	95(2)	C(26)	B(1)	C(40)	110.4(6)
C(51)	C(53)	C(54)	137(2)	C(39)	B(1)	C(40)	105.3(5)
C(52)	C(53)	C(54)	89(2)	C(53)	C(54)	C(55)	97(3)
C(54)	C(55)	C(56)	169(4)	C(54)	C(55)	C(57)	120(3)
C(54)	C(55)	C(58)	103(3)	C(56)	C(55)	C(57)	66(2)
C(56)	C(55)	C(58)	77(3)	C(57)	C(55)	C(58)	38(1)
C(55)	C(56)	C(57)	88(3)	C(55)	C(56)	C(58)	79(3)
C(57)	C(56)	C(58)	39(1)	C(55)	C(57)	C(56)	25.6(9)
C(55)	C(57)	C(58)	77(2)	C(56)	C(57)	C(58)	82(2)
C(50)	C(58)	C(55)	130(3)	C(50)	C(58)	C(56)	130(3)
C(50)	C(58)	C(57)	161(4)	C(55)	C(58)	C(56)	23(1)
C(55)	C(58)	C(57)	65(2)				

Angles are in degrees. Estimated standard deviations in the least significant figure are given in parentheses.

Table 12. Anisotropic Displacement Parameters for **4**.

atom	U11	U22	U33	U12	U13	U23
Ir(01)	0.0248(2)	0.0190(1)	0.0180(1)	0.0005(2)	0.0036(1)	-0.0005(2)
Cl(1)	0.212(6)	0.056(2)	0.108(3)	0.001(3)	0.059(4)	-0.003(2)
Cl(2)	0.149(4)	0.121(3)	0.114(3)	0.067(3)	0.051(3)	0.018(2)
P(1)	0.029(1)	0.0203(8)	0.0187(9)	0.001(1)	0.0043(8)	-0.0013(9)
P(2)	0.030(1)	0.024(1)	0.020(1)	0.0045(8)	0.0080(8)	0.0031(8)
P(3)	0.026(1)	0.0220(9)	0.019(1)	0.0023(8)	0.0029(8)	0.0012(8)
P(4)	0.031(1)	0.026(1)	0.026(1)	-0.0012(9)	0.002(1)	-0.0051(8)
C(1)	0.020(4)	0.034(4)	0.021(4)	0.003(3)	0.003(3)	-0.001(3)
C(2)	0.038(5)	0.021(4)	0.028(4)	-0.001(3)	0.005(4)	-0.002(3)
C(3)	0.044(5)	0.017(4)	0.048(5)	-0.002(3)	0.008(4)	0.008(4)
C(4)	0.049(6)	0.023(4)	0.037(5)	0.002(4)	0.010(4)	0.014(4)
C(5)	0.040(5)	0.040(4)	0.023(4)	0.007(4)	0.006(4)	0.002(4)
C(6)	0.032(5)	0.017(4)	0.032(4)	0.002(3)	0.010(4)	0.008(3)
C(7)	0.048(5)	0.028(4)	0.018(4)	0.014(4)	0.008(4)	0.009(3)
C(8)	0.042(6)	0.044(5)	0.026(4)	0.002(4)	0.004(4)	-0.003(3)
C(9)	0.039(6)	0.095(8)	0.032(5)	0.002(6)	0.000(4)	0.001(6)
C(10)	0.041(7)	0.093(8)	0.054(6)	0.035(6)	0.019(5)	0.022(6)
C(11)	0.077(8)	0.055(6)	0.061(7)	0.035(6)	0.039(6)	0.017(5)
C(12)	0.049(6)	0.043(5)	0.055(6)	0.021(4)	0.029(5)	0.009(4)
C(13)	0.044(5)	0.022(4)	0.014(3)	0.006(4)	-0.001(3)	-0.007(3)
C(14)	0.018(4)	0.025(4)	0.042(5)	-0.000(3)	0.004(4)	0.003(4)
C(15)	0.027(5)	0.028(4)	0.034(5)	-0.002(3)	0.001(4)	-0.003(3)
C(16)	0.040(6)	0.047(5)	0.040(5)	-0.007(4)	-0.002(4)	0.018(4)
C(17)	0.038(6)	0.035(5)	0.073(7)	0.001(4)	-0.000(5)	0.015(5)
C(18)	0.054(6)	0.032(5)	0.057(6)	0.009(4)	0.003(5)	-0.004(4)
C(19)	0.046(6)	0.027(4)	0.037(5)	0.007(4)	0.008(4)	-0.000(4)
C(20)	0.026(4)	0.024(3)	0.025(4)	0.003(4)	0.010(3)	-0.003(4)
C(21)	0.026(4)	0.050(5)	0.033(4)	-0.002(4)	0.005(4)	-0.004(4)
C(22)	0.033(5)	0.057(5)	0.045(5)	0.002(5)	0.017(4)	-0.004(5)
C(23)	0.057(6)	0.045(5)	0.049(6)	-0.003(5)	0.037(5)	-0.006(5)
C(24)	0.049(6)	0.048(5)	0.028(4)	0.002(5)	0.017(4)	-0.005(4)
C(25)	0.028(4)	0.028(4)	0.030(4)	-0.001(4)	0.005(3)	-0.003(4)
C(26)	0.031(5)	0.015(3)	0.024(4)	-0.002(3)	0.004(3)	0.002(3)
C(27)	0.037(5)	0.019(4)	0.029(4)	0.005(3)	0.012(4)	0.004(3)
C(28)	0.045(6)	0.034(4)	0.034(5)	-0.004(4)	0.011(4)	0.004(4)
C(29)	0.035(6)	0.065(6)	0.045(6)	-0.011(4)	0.017(5)	0.007(5)
C(30)	0.060(7)	0.063(6)	0.041(6)	-0.003(5)	0.022(5)	0.017(5)
C(31)	0.063(7)	0.060(6)	0.026(5)	0.006(5)	0.012(5)	0.003(4)
C(32)	0.046(6)	0.041(5)	0.029(5)	-0.004(4)	0.004(4)	0.002(4)
C(33)	0.028(5)	0.027(4)	0.023(4)	-0.000(3)	0.001(3)	0.001(3)
C(34)	0.036(6)	0.036(5)	0.091(8)	0.005(4)	0.003(5)	0.012(5)
C(35)	0.021(6)	0.055(6)	0.15(1)	0.005(5)	-0.006(6)	0.019(7)
C(36)	0.049(7)	0.041(5)	0.069(7)	0.010(5)	-0.018(5)	0.010(5)
C(37)	0.056(7)	0.023(4)	0.074(7)	0.015(5)	-0.012(5)	0.001(4)
C(38)	0.039(5)	0.029(4)	0.061(6)	-0.001(4)	-0.007(5)	0.006(4)
C(39)	0.029(5)	0.022(4)	0.024(4)	0.002(3)	0.008(4)	0.005(3)
C(40)	0.032(5)	0.026(4)	0.022(4)	0.003(4)	-0.008(4)	0.004(3)
C(41)	0.052(6)	0.031(4)	0.039(5)	0.009(4)	0.004(4)	-0.011(4)
C(42)	0.057(7)	0.030(4)	0.047(6)	0.005(4)	-0.002(5)	-0.019(4)
C(43)	0.080(8)	0.021(4)	0.049(6)	-0.006(5)	-0.016(5)	-0.001(4)
C(44)	0.050(6)	0.028(4)	0.048(5)	-0.003(4)	-0.000(5)	0.007(4)
C(45)	0.042(6)	0.026(4)	0.034(5)	0.003(4)	-0.007(4)	-0.002(4)
C(46)	0.034(5)	0.040(5)	0.026(4)	-0.002(4)	-0.001(4)	-0.010(3)
C(47)	0.042(5)	0.032(4)	0.026(4)	-0.001(4)	0.003(4)	-0.008(3)
C(48)	0.049(6)	0.037(5)	0.044(5)	-0.011(4)	0.003(5)	-0.006(4)

Table 13. Positional parameters and B(eq) for **8**.

atom	x	y	z	B(eq)
Ir(1)	0.5731(1)	0.49808(9)	0.58508(8)	1.34(4)
P(1)	0.6298(5)	0.5845(4)	0.7381(4)	1.3(2)
P(2)	0.7642(5)	0.6263(4)	0.5538(4)	1.5(2)
P(3)	0.6579(5)	0.3807(4)	0.6487(4)	1.6(2)
C(1)	0.992(2)	0.632(2)	0.815(1)	1.2(4)
C(2)	1.026(2)	0.567(2)	0.881(1)	1.8(5)
C(3)	1.135(2)	0.614(2)	0.946(2)	2.7(5)
C(4)	1.212(2)	0.725(2)	0.956(2)	2.7(5)
C(5)	1.180(2)	0.794(2)	0.888(2)	2.5(5)
C(6)	1.072(2)	0.744(2)	0.824(2)	2.2(5)
C(7)	0.786(2)	0.651(1)	0.776(1)	1.1(4)
C(8)	0.889(2)	0.613(2)	0.635(1)	1.4(4)
C(9)	0.788(2)	0.450(1)	0.743(1)	1.2(4)
C(10)	0.571(2)	0.684(1)	0.767(1)	1.1(4)
C(11)	0.450(2)	0.654(2)	0.752(1)	2.1(5)
C(12)	0.399(2)	0.720(2)	0.786(1)	2.1(5)
C(13)	0.468(2)	0.821(2)	0.833(1)	1.5(4)
C(14)	0.592(2)	0.860(2)	0.845(1)	2.6(5)
C(15)	0.642(2)	0.789(2)	0.812(1)	1.6(5)
C(16)	0.575(2)	0.486(2)	0.829(1)	2.1(5)
C(17)	0.457(2)	0.402(2)	0.810(1)	2.0(5)
C(18)	0.415(2)	0.336(2)	0.879(2)	2.5(5)
C(19)	0.487(2)	0.351(2)	0.967(1)	2.0(5)
C(20)	0.601(2)	0.432(2)	0.987(1)	1.9(5)
C(21)	0.645(2)	0.502(2)	0.918(1)	1.6(4)
C(22)	0.800(2)	0.774(1)	0.575(1)	0.9(4)
C(23)	0.709(2)	0.812(2)	0.584(1)	1.9(5)
C(24)	0.731(2)	0.925(2)	0.600(1)	2.0(5)
C(25)	0.850(2)	1.007(2)	0.606(2)	2.9(5)
C(26)	0.940(2)	0.974(2)	0.598(1)	2.4(5)
C(27)	0.914(2)	0.861(2)	0.581(1)	1.7(4)
C(28)	0.802(2)	0.622(1)	0.434(1)	0.4(4)
C(29)	0.816(2)	0.706(2)	0.378(1)	2.2(5)
C(30)	0.857(2)	0.705(2)	0.292(1)	2.4(5)
C(31)	0.882(2)	0.616(2)	0.267(1)	2.0(5)
C(32)	0.863(2)	0.525(2)	0.322(1)	2.1(5)
C(33)	0.827(2)	0.531(2)	0.407(1)	2.0(5)
C(34)	0.706(2)	0.311(1)	0.561(1)	0.9(4)
C(35)	0.821(2)	0.321(1)	0.569(1)	1.5(4)
C(36)	0.850(2)	0.265(2)	0.504(1)	1.7(4)
C(37)	0.765(2)	0.193(2)	0.432(1)	1.9(5)
C(38)	0.647(2)	0.178(2)	0.422(1)	2.0(5)
C(39)	0.620(2)	0.240(2)	0.488(2)	2.5(5)
C(40)	0.554(2)	0.256(2)	0.693(1)	1.8(5)
C(41)	0.435(2)	0.203(2)	0.650(2)	2.2(5)
C(42)	0.355(2)	0.106(2)	0.681(2)	2.5(5)
C(43)	0.397(2)	0.062(2)	0.758(2)	2.8(5)
C(44)	0.514(2)	0.115(2)	0.800(1)	2.5(5)
C(45)	0.593(2)	0.209(2)	0.772(2)	2.6(5)
C(46)	0.957(3)	0.771(2)	1.050(2)	3(1)

C(47)	0.871(3)	0.812(3)	1.038(2)	3(1)
C(48)	0.894(3)	0.914(3)	1.083(2)	5(2)
C(49)	1.002(4)	0.978(2)	1.141(3)	6(2)
C(50)	1.082(3)	0.932(3)	1.153(2)	6(2)
C(51)	1.066(2)	0.832(3)	1.108(2)	4(1)
B(1)	0.866(2)	0.585(2)	0.744(2)	0.6(5)

Table 14. Intramolecular Distances Involving the Nonhydrogen Atoms for **8**.

atom	atom	distance	ADC(*)	atom	atom	distance	ADC(*)
Ir(1)	Ir(1)	2.796(2)	66602	C(12)	C(13)	1.33(2)	1
Ir(1)	P(1)	2.298(6)	1	C(13)	C(14)	1.40(3)	1
Ir(1)	P(2)	2.415(6)	1	C(14)	C(15)	1.41(2)	1
Ir(1)	P(3)	2.309(6)	1	C(16)	C(17)	1.40(2)	1
P(1)	C(7)	1.75(2)	1	C(16)	C(21)	1.37(2)	1
P(1)	C(10)	1.79(2)	1	C(17)	C(18)	1.36(2)	1
P(1)	C(16)	1.87(2)	1	C(18)	C(19)	1.38(3)	1
P(2)	C(8)	1.85(2)	1	C(19)	C(20)	1.35(3)	1
P(2)	C(22)	1.79(2)	1	C(20)	C(21)	1.40(2)	1
P(2)	C(28)	1.86(2)	1	C(22)	C(23)	1.44(2)	1
P(3)	C(9)	1.80(2)	1	C(22)	C(27)	1.39(2)	1
P(3)	C(34)	1.84(2)	1	C(23)	C(24)	1.38(2)	1
P(3)	C(40)	1.83(2)	1	C(24)	C(25)	1.41(3)	1
C(1)	C(2)	1.41(2)	1	C(25)	C(26)	1.38(2)	1
C(1)	C(6)	1.38(2)	1	C(26)	C(27)	1.37(2)	1
C(1)	B(1)	1.58(3)	1	C(28)	C(29)	1.35(2)	1
C(2)	C(3)	1.39(3)	1	C(28)	C(33)	1.40(2)	1
C(3)	C(4)	1.35(3)	1	C(29)	C(30)	1.42(2)	1
C(4)	C(5)	1.45(3)	1	C(30)	C(31)	1.37(2)	1
C(5)	C(6)	1.38(3)	1	C(31)	C(32)	1.41(2)	1
C(7)	B(1)	1.66(3)	1	C(32)	C(33)	1.38(2)	1
C(8)	B(1)	1.67(3)	1	C(34)	C(35)	1.37(2)	1
C(9)	B(1)	1.63(3)	1	C(34)	C(39)	1.37(2)	1
C(10)	C(11)	1.37(2)	1	C(35)	C(36)	1.35(2)	1
C(10)	C(15)	1.36(2)	1	C(36)	C(37)	1.35(2)	1
C(11)	C(12)	1.39(2)	1	C(37)	C(38)	1.38(2)	1
C(38)	C(39)	1.41(2)	1	C(40)	C(41)	1.37(3)	1
C(40)	C(45)	1.41(3)	1	C(41)	C(42)	1.39(2)	1
C(42)	C(43)	1.38(3)	1	C(43)	C(44)	1.35(3)	1
C(44)	C(45)	1.35(2)	1	C(46)	C(47)	1.37(3)	1
C(46)	C(51)	1.36(3)	1	C(47)	C(48)	1.36(3)	1
C(48)	C(49)	1.37(4)	1	C(49)	C(50)	1.34(4)	1
C(50)	C(51)	1.37(3)	1				

Distances are in angstroms. Estimated standard deviations in the least significant figure are given in parentheses.

Table 15. Intramolecular Bond Angles Involving the Nonhydrogen Atoms

atom	atom	atom	angle	atom	atom	atom	angle
Ir(1)	Ir(1)	P(1)	137.3(1)	C(6)	C(1)	B(1)	121(2)
Ir(1)	Ir(1)	P(2)	98.2(1)	C(1)	C(2)	C(3)	121(2)
Ir(1)	Ir(1)	P(3)	137.3(2)	C(2)	C(3)	C(4)	124(2)
P(1)	Ir(1)	P(2)	89.5(2)	C(3)	C(4)	C(5)	116(2)
P(1)	Ir(1)	P(3)	84.1(2)	C(4)	C(5)	C(6)	118(2)
P(2)	Ir(1)	P(3)	90.5(2)	C(1)	C(6)	C(5)	125(2)
Ir(1)	P(1)	C(7)	112.1(6)	P(1)	C(7)	B(1)	118(1)
Ir(1)	P(1)	C(10)	118.3(7)	P(2)	C(8)	B(1)	115(1)
Ir(1)	P(1)	C(16)	114.3(6)	P(3)	C(9)	B(1)	118(1)
C(7)	P(1)	C(10)	107.4(9)	P(1)	C(10)	C(11)	121(2)
C(7)	P(1)	C(16)	105.5(9)	P(1)	C(10)	C(15)	123(2)
C(10)	P(1)	C(16)	97.8(8)	C(11)	C(10)	C(15)	115(2)
Ir(1)	P(2)	C(8)	110.9(6)	C(10)	C(11)	C(12)	124(2)
Ir(1)	P(2)	C(22)	115.9(7)	C(11)	C(12)	C(13)	121(2)
Ir(1)	P(2)	C(28)	121.6(6)	C(12)	C(13)	C(14)	118(2)
C(8)	P(2)	C(22)	102.3(9)	C(13)	C(14)	C(15)	120(2)
C(8)	P(2)	C(28)	103.8(9)	C(10)	C(15)	C(14)	122(2)
C(22)	P(2)	C(28)	99.9(8)	P(1)	C(16)	C(17)	120(2)
Ir(1)	P(3)	C(9)	114.4(6)	P(1)	C(16)	C(21)	121(2)
Ir(1)	P(3)	C(34)	113.8(6)	C(17)	C(16)	C(21)	119(2)
Ir(1)	P(3)	C(40)	114.4(7)	C(16)	C(17)	C(18)	119(2)
C(9)	P(3)	C(34)	105.5(9)	C(17)	C(18)	C(19)	121(2)
C(9)	P(3)	C(40)	107.5(9)	C(18)	C(19)	C(20)	120(2)
C(34)	P(3)	C(40)	99.8(8)	C(19)	C(20)	C(21)	120(2)
C(2)	C(1)	C(6)	115(2)	C(16)	C(21)	C(20)	121(2)
C(2)	C(1)	B(1)	124(2)	P(2)	C(22)	C(23)	121(1)
P(2)	C(22)	C(27)	125(2)	C(40)	C(41)	C(42)	123(2)
C(23)	C(22)	C(27)	114(2)	C(41)	C(42)	C(43)	119(2)
C(22)	C(23)	C(24)	124(2)	C(42)	C(43)	C(44)	118(2)
C(23)	C(24)	C(25)	118(2)	C(43)	C(44)	C(45)	124(2)
C(24)	C(25)	C(26)	120(2)	C(40)	C(45)	C(44)	120(2)
C(25)	C(26)	C(27)	120(2)	C(47)	C(46)	C(51)	121(2)
C(22)	C(27)	C(26)	124(2)	C(46)	C(47)	C(48)	120(3)
P(2)	C(28)	C(29)	123(1)	C(47)	C(48)	C(49)	121(3)
P(2)	C(28)	C(33)	117(1)	C(48)	C(49)	C(50)	116(3)
C(29)	C(28)	C(33)	120(2)	C(49)	C(50)	C(51)	125(3)
C(28)	C(29)	C(30)	121(2)	C(46)	C(51)	C(50)	116(3)
C(29)	C(30)	C(31)	118(2)	C(1)	B(1)	C(7)	109(2)
C(30)	C(31)	C(32)	121(2)	C(1)	B(1)	C(8)	109(2)
C(31)	C(32)	C(33)	118(2)	C(1)	B(1)	C(9)	113(2)
C(28)	C(33)	C(32)	121(2)	C(7)	B(1)	C(8)	109(2)
P(3)	C(34)	C(35)	124(2)	C(7)	B(1)	C(9)	108(2)
P(3)	C(34)	C(39)	118(2)	C(8)	B(1)	C(9)	108(2)
C(35)	C(34)	C(39)	118(2)	C(34)	C(35)	C(36)	121(2)
C(35)	C(36)	C(37)	121(2)	C(36)	C(37)	C(38)	120(2)
C(37)	C(38)	C(39)	118(2)	C(34)	C(39)	C(38)	122(2)
P(3)	C(40)	C(41)	122(2)				
P(3)	C(40)	C(45)	121(2)				
C(41)	C(40)	C(45)	117(2)				

Angles are in degrees. Estimated standard deviations in the least significant figure are given in parentheses.

Table 16. Anisotropic displacement parameters for **8**.

atom	U11	U22	U33	U12	U13	U23
Ir(1)	0.0144(6)	0.0237(5)	0.0149(6)	0.0087(4)	0.0056(4)	0.0085(4)
P(1)	0.002(4)	0.013(3)	0.029(4)	-0.000(3)	0.000(3)	0.011(3)
P(2)	0.020(4)	0.017(4)	0.023(4)	0.008(3)	0.007(4)	0.005(3)
P(3)	0.021(4)	0.020(4)	0.026(4)	0.013(3)	0.009(4)	0.007(3)
C(46)	0.05(2)	0.04(2)	0.02(2)	0.01(2)	0.02(2)	0.00(1)
C(47)	0.04(2)	0.06(2)	0.02(2)	0.01(2)	0.01(2)	-0.00(2)
C(48)	0.10(3)	0.06(2)	0.03(2)	0.04(2)	0.03(2)	0.03(2)
C(49)	0.14(4)	0.02(2)	0.10(3)	0.02(2)	0.10(3)	0.01(2)
C(50)	0.08(3)	0.05(2)	0.04(2)	-0.04(2)	0.03(2)	-0.04(2)
C(51)	0.01(2)	0.09(2)	0.06(2)	0.03(2)	0.02(2)	0.01(2)

Table 17. Positional parameters and B(eq) for **10**.

atom	x	y	z	B(eq)
Ir(1)	0.88473(3)	-0.14401(1)	0.64154(4)	1.20(2)
I(1)	0.88994(6)	-0.17841(2)	0.83805(6)	2.13(3)
I(2)	1.06938(6)	-0.18459(2)	0.61119(6)	2.00(3)
P(1)	0.7280(2)	-0.10968(8)	0.6896(2)	1.3(1)
P(2)	0.8018(2)	-0.15844(8)	0.4787(2)	1.2(1)
P(3)	0.9501(2)	-0.08718(8)	0.5637(2)	1.2(1)
C(1)	0.7046(8)	-0.0663(3)	0.6009(8)	1.1(2)
C(2)	0.6056(8)	-0.1408(3)	0.6817(8)	1.7(2)
C(3)	0.5060(8)	-0.1215(3)	0.6542(9)	1.8(2)
C(4)	0.4125(9)	-0.1442(4)	0.650(1)	2.5(2)
C(5)	0.417(1)	-0.1852(3)	0.675(1)	2.3(2)
C(6)	0.5109(8)	-0.2036(3)	0.7010(9)	1.7(2)
C(7)	0.6045(8)	-0.1814(3)	0.7063(8)	1.7(2)
C(8)	0.7241(8)	-0.0915(3)	0.8315(8)	1.1(2)
C(9)	0.7643(9)	-0.0539(3)	0.859(1)	2.0(2)
C(10)	0.7618(9)	-0.0409(3)	0.9665(9)	1.8(2)
C(11)	0.7248(9)	-0.0656(3)	1.0467(9)	2.0(2)
C(12)	0.6840(9)	-0.1033(3)	1.020(1)	2.2(2)
C(13)	0.6829(8)	-0.1167(3)	0.9119(9)	1.7(2)
C(14)	0.7014(8)	-0.1211(3)	0.4382(8)	1.3(2)
C(15)	0.8760(8)	-0.1675(3)	0.3545(9)	1.5(2)
C(16)	0.8678(8)	-0.1423(3)	0.2644(8)	1.4(2)
C(17)	0.9242(9)	-0.1512(3)	0.1699(9)	2.1(2)
C(18)	0.9863(9)	-0.1855(3)	0.1651(9)	2.0(2)
C(19)	0.9909(9)	-0.2118(3)	0.251(1)	2.0(2)
C(20)	0.9368(8)	-0.2033(3)	0.3478(9)	1.6(2)
C(21)	0.7377(8)	-0.2080(3)	0.4981(8)	1.3(2)
C(22)	0.6415(9)	-0.2158(3)	0.4410(9)	1.8(2)
C(23)	0.589(1)	-0.2525(3)	0.459(1)	2.2(2)
C(24)	0.631(1)	-0.2804(3)	0.530(1)	2.4(2)
C(25)	0.7265(9)	-0.2733(3)	0.5855(9)	1.9(2)
C(26)	0.7815(8)	-0.2369(3)	0.5691(9)	1.6(2)
C(27)	0.8652(8)	-0.0654(3)	0.4594(8)	1.2(2)
C(28)	1.0830(8)	-0.0881(3)	0.5053(8)	1.3(2)
C(29)	1.0995(8)	-0.1116(3)	0.4125(9)	1.7(2)
C(30)	1.1987(8)	-0.1105(3)	0.3621(8)	1.5(2)
C(31)	1.2789(8)	-0.0856(3)	0.4015(9)	1.7(2)
C(32)	1.2632(9)	-0.0626(3)	0.4926(9)	1.7(2)
C(33)	1.1681(8)	-0.0645(3)	0.5452(8)	1.4(2)
C(34)	0.9698(8)	-0.0511(3)	0.6746(8)	1.3(2)
C(35)	1.0208(8)	-0.0628(3)	0.7704(9)	1.6(2)
C(36)	1.0457(9)	-0.0360(3)	0.8518(9)	1.9(2)
C(37)	1.0149(8)	0.0043(3)	0.8409(8)	1.6(2)
C(38)	0.9648(9)	0.0174(3)	0.7457(9)	1.8(2)
C(39)	0.9423(8)	-0.0097(3)	0.6627(8)	1.3(2)
C(40)	0.6659(8)	-0.0433(3)	0.3946(8)	1.1(2)
C(41)	0.5553(8)	-0.0409(3)	0.4018(9)	1.6(2)
C(42)	0.4946(9)	-0.0145(3)	0.337(1)	2.1(2)
C(43)	0.5450(9)	0.0107(3)	0.264(1)	2.2(2)
C(44)	0.6529(9)	0.0089(3)	0.2528(9)	1.8(2)
C(45)	0.7121(8)	-0.0179(3)	0.3166(8)	1.6(2)

C(46)	0.259(2)	-0.2434(7)	0.380(2)	9(1)
C(47)	0.311(1)	-0.2160(5)	0.307(1)	5(1)
C(48)	0.285(1)	-0.2154(4)	0.195(1)	3.4(7)
C(49)	0.338(1)	-0.1877(4)	0.133(1)	4.6(8)
C(50)	0.414(1)	-0.1605(6)	0.173(2)	7(1)
C(51)	0.433(2)	-0.1618(7)	0.278(2)	8(1)
C(52)	0.384(1)	-0.1879(6)	0.353(1)	5(1)
C(53)	0.426(1)	-0.0481(4)	0.031(1)	3.4(7)
C(54)	0.335(1)	-0.0757(3)	0.009(1)	2.2(6)
C(55)	0.249(1)	-0.0769(3)	0.080(1)	2.1(6)
C(56)	0.163(1)	-0.1019(4)	0.060(1)	3.4(7)
C(57)	0.160(1)	-0.1261(4)	-0.028(1)	3.2(7)
C(58)	0.244(1)	-0.1257(4)	-0.101(1)	4.0(7)
C(59)	0.331(1)	-0.1007(3)	-0.0822(9)	2.4(6)
B(1)	0.736(1)	-0.0738(3)	0.472(1)	1.2(2)

Table 18. Intramolecular Distances Involving the Nonhydrogen Atoms for **10**

atom	atom	distance	atom	atom	distance
Ir(1)	I(1)	2.6697(8)	C(12)	C(13)	1.40(1)
Ir(1)	I(2)	2.7086(8)	C(14)	B(1)	1.67(1)
Ir(1)	P(1)	2.357(3)	C(15)	C(16)	1.39(1)
Ir(1)	P(2)	2.280(3)	C(15)	C(20)	1.41(1)
Ir(1)	P(3)	2.274(3)	C(16)	C(17)	1.41(1)
P(1)	C(1)	1.82(1)	C(17)	C(18)	1.38(1)
P(1)	C(2)	1.85(1)	C(18)	C(19)	1.37(1)
P(1)	C(8)	1.85(1)	C(19)	C(20)	1.41(1)
P(2)	C(14)	1.82(1)	C(21)	C(22)	1.40(1)
P(2)	C(15)	1.83(1)	C(21)	C(26)	1.40(1)
P(2)	C(21)	1.85(1)	C(22)	C(23)	1.40(1)
P(3)	C(27)	1.79(1)	C(23)	C(24)	1.37(2)
P(3)	C(28)	1.83(1)	C(24)	C(25)	1.38(2)
P(3)	C(34)	1.82(1)	C(25)	C(26)	1.41(1)
C(1)	B(1)	1.66(2)	C(27)	B(1)	1.66(2)
C(2)	C(3)	1.43(1)	C(28)	C(29)	1.40(1)
C(2)	C(7)	1.38(1)	C(28)	C(33)	1.40(1)
C(3)	C(4)	1.39(1)	C(29)	C(30)	1.40(1)
C(4)	C(5)	1.40(2)	C(30)	C(31)	1.38(1)
C(5)	C(6)	1.36(1)	C(31)	C(32)	1.37(1)
C(6)	C(7)	1.38(1)	C(32)	C(33)	1.37(1)
C(8)	C(9)	1.38(1)	C(34)	C(35)	1.38(1)
C(8)	C(13)	1.40(1)	C(34)	C(39)	1.42(1)
C(9)	C(10)	1.40(1)	C(35)	C(36)	1.37(1)
C(10)	C(11)	1.37(1)	C(36)	C(37)	1.40(1)
C(11)	C(12)	1.38(1)	C(37)	C(38)	1.38(1)
C(38)	C(39)	1.38(1)	C(40)	C(41)	1.39(1)
C(40)	C(45)	1.41(1)	C(40)	B(1)	1.62(1)
C(41)	C(42)	1.39(1)	C(42)	C(43)	1.40(1)
C(43)	C(44)	1.36(1)	C(44)	C(45)	1.39(1)
C(46)	C(47)	1.45(2)	C(47)	C(48)	1.40(2)
C(47)	C(52)	1.41(2)	C(48)	C(49)	1.38(2)
C(49)	C(50)	1.39(2)	C(50)	C(51)	1.30(3)
C(51)	C(52)	1.42(3)	C(53)	C(54)	1.48(2)
C(54)	C(55)	1.41(2)	C(54)	C(59)	1.39(2)
C(55)	C(56)	1.37(2)	C(56)	C(57)	1.34(2)
C(57)	C(58)	1.39(2)	C (58)	C(59)	1.39(2)

Distances are in angstroms. Estimated standard deviations in the least significant figure are given in parentheses.

Table 19. Intramolecular Bond Angles Involving the Nonhydrogen Atoms for **10**.

atom	atom	atom	angle	atom	atom	atom	angle
I(1)	Ir(1)	I(2)	84.98(3)	C(27)	P(3)	C(34)	109.6(5)
I(1)	Ir(1)	P(1)	88.83(7)	C(28)	P(3)	C(34)	101.4(5)
I(1)	Ir(1)	P(2)	134.74(7)	P(1)	C(1)	B(1)	114.5(7)
I(1)	Ir(1)	P(3)	137.20(7)	P(1)	C(2)	C(3)	118.7(8)
I(2)	Ir(1)	P(1)	173.40(7)	P(1)	C(2)	C(7)	123.1(8)
I(2)	Ir(1)	P(2)	98.34(7)	C(3)	C(2)	C(7)	118(1)
I(2)	Ir(1)	P(3)	91.99(7)	C(2)	C(3)	C(4)	120(1)
P(1)	Ir(1)	P(2)	87.6(1)	C(3)	C(4)	C(5)	119(1)
P(1)	Ir(1)	P(3)	91.01(9)	C(4)	C(5)	C(6)	121(1)
P(2)	Ir(1)	P(3)	88.0(1)	C(5)	C(6)	C(7)	120(1)
Ir(1)	P(1)	C(1)	110.6(3)	C(2)	C(7)	C(6)	121(1)
Ir(1)	P(1)	C(2)	114.4(3)	P(1)	C(8)	C(9)	120.2(8)
Ir(1)	P(1)	C(8)	115.9(3)	P(1)	C(8)	C(13)	119.4(7)
C(1)	P(1)	C(2)	106.8(5)	C(9)	C(8)	C(13)	120(1)
C(1)	P(1)	C(8)	107.4(4)	C(8)	C(9)	C(10)	119(1)
C(2)	P(1)	C(8)	100.9(5)	C(9)	C(10)	C(11)	121(1)
Ir(1)	P(2)	C(14)	113.0(3)	C(10)	C(11)	C(12)	120(1)
Ir(1)	P(2)	C(15)	122.4(4)	C(11)	C(12)	C(13)	120(1)
Ir(1)	P(2)	C(21)	105.2(3)	C(8)	C(13)	C(12)	119.0(9)
C(14)	P(2)	C(15)	104.2(5)	P(2)	C(14)	B(1)	113.5(7)
C(14)	P(2)	C(21)	109.9(5)	P(2)	C(15)	C(16)	122.4(8)
C(15)	P(2)	C(21)	101.1(5)	P(2)	C(15)	C(20)	118.2(8)
Ir(1)	P(3)	C(27)	114.9(3)	C(16)	C(15)	C(20)	119.2(9)
Ir(1)	P(3)	C(28)	119.5(3)	C(15)	C(16)	C(17)	120.2(9)
Ir(1)	P(3)	C(34)	105.7(3)	C(16)	C(17)	C(18)	120(1)
C(27)	P(3)	C(28)	104.7(5)	C(17)	C(18)	C(19)	120(1)
C(18)	C(19)	C(20)	121(1)	C(34)	C(39)	C(38)	120.4(9)
C(15)	C(20)	C(19)	119(1)	C(41)	C(40)	C(45)	115.8(9)
P(2)	C(21)	C(22)	118.1(8)	C(41)	C(40)	B(1)	121.3(9)
P(2)	C(21)	C(26)	121.6(8)	C(45)	C(40)	B(1)	122.9(9)
C(22)	C(21)	C(26)	120.3(9)	C(40)	C(41)	C(42)	122(1)
C(21)	C(22)	C(23)	119(1)	C(41)	C(42)	C(43)	120(1)
C(22)	C(23)	C(24)	121(1)	C(42)	C(43)	C(44)	120(1)
C(23)	C(24)	C(25)	121(1)	C(43)	C(44)	C(45)	119(1)
C(24)	C(25)	C(26)	120(1)	C(40)	C(45)	C(44)	123(1)
C(21)	C(26)	C(25)	119(1)	C(46)	C(47)	C(48)	121(2)
P(3)	C(27)	B(1)	115.4(7)	C(46)	C(47)	C(52)	117(2)
P(3)	C(28)	C(29)	118.9(8)	C(48)	C(47)	C(52)	121(2)
P(3)	C(28)	C(33)	123.0(8)	C(47)	C(48)	C(49)	117(1)
C(29)	C(28)	C(33)	117.9(9)	C(48)	C(49)	C(50)	125(2)
C(28)	C(29)	C(30)	119.9(9)	C(49)	C(50)	C(51)	116(2)
C(29)	C(30)	C(31)	120.3(9)	C(50)	C(51)	C(52)	126(2)
C(30)	C(31)	C(32)	120(1)	C(47)	C(52)	C(51)	116(2)
C(31)	C(32)	C(33)	120(1)	C(53)	C(54)	C(55)	120(1)
C(28)	C(33)	C(32)	122(1)	C(53)	C(54)	C(59)	122(1)
P(3)	C(34)	C(35)	120.3(7)	C(55)	C(54)	C(59)	118(1)
P(3)	C(34)	C(39)	121.8(8)	C(54)	C(55)	C(56)	121(1)
C(35)	C(34)	C(39)	117.6(9)	C(55)	C(56)	C(57)	121(1)

C(34)	C(35)	C(36)	122(1)	C(56)	C(57)	C(58)	120(1)
C(35)	C(36)	C(37)	120(1)	C(57)	C(58)	C(59)	120(1)
C(36)	C(37)	C(38)	120(1)	C(54)	C(59)	C(58)	120(1)
C(37)	C(38)	C(39)	120.1(9)	C(1)	B(1)	C(14)	108.1(8)
C(1)	B(1)	C(27)	108.4(9)	C(1)	B(1)	C(40)	109.3(8)
C(14)	B(1)	C(27)	112.3(8)	C(14)	B(1)	C(40)	108.0(8)
C(27)	B(1)	C(40)	110.7(8)				

Table 20. Anisotropic displacement values for **10**.

atom	U11	U22	U33	U12	U13	U23
Ir(1)	0.0161(2)	0.0127(2)	0.0169(2)	0.0006(2)	0.0009(2)	0.0010(2)
I(1)	0.0341(5)	0.0252(4)	0.0217(4)	0.0066(4)	0.0026(3)	0.0056(3)
I(2)	0.0213(4)	0.0220(4)	0.0329(5)	0.0050(3)	0.0051(3)	0.0069(3)
P(1)	0.017(2)	0.014(1)	0.018(2)	-0.003(1)	0.002(1)	0.000(1)
P(2)	0.016(2)	0.010(1)	0.021(2)	0.000(1)	0.002(1)	0.000(1)
P(3)	0.013(2)	0.015(1)	0.017(2)	0.001(1)	0.002(1)	-0.000(1)
C(46)	0.11(2)	0.14(2)	0.09(2)	0.09(1)	0.04(1)	0.03(1)
C(47)	0.07(1)	0.06(1)	0.06(1)	0.04(1)	-0.00(1)	-0.01(1)
C(48)	0.05(1)	0.021(7)	0.06(1)	0.026(7)	-0.006(8)	-0.007(7)
C(49)	0.04(1)	0.040(9)	0.09(1)	0.020(8)	0.01(1)	-0.01(1)
C(50)	0.05(1)	0.07(1)	0.14(2)	0.03(1)	0.04(1)	0.01(1)
C(51)	0.08(2)	0.10(2)	0.12(2)	0.07(1)	-0.05(1)	-0.04(2)
C(52)	0.06(1)	0.07(1)	0.07(1)	0.05(1)	-0.03(1)	-0.03(1)
C(53)	0.047(9)	0.041(8)	0.041(9)	-0.009(7)	0.013(7)	0.004(6)
C(54)	0.031(8)	0.016(6)	0.036(8)	-0.005(5)	-0.012(6)	0.013(6)
C(55)	0.031(8)	0.020(6)	0.027(7)	0.001(5)	-0.006(6)	-0.003(5)
C(56)	0.029(8)	0.052(9)	0.05(1)	-0.004(7)	-0.001(7)	0.010(8)
C(57)	0.05(1)	0.027(7)	0.04(1)	-0.017(6)	-0.013(8)	0.008(6)
C(58)	0.09(1)	0.036(8)	0.023(8)	-0.002(8)	-0.022(8)	-0.003(6)
C(59)	0.051(9)	0.028(7)	0.015(7)	-0.010(6)	0.001(6)	0.003(5)

Table 21. Positional parameters and B(eq) for **13**.

atom	x	y	z	B(eq)
Ir(1)	0.7011(2)	0.9335(2)	0.70871(8)	1.64(5)
Cl(1)	0.840(1)	1.1288(8)	0.6766(4)	4.1(3)
Cl(2)	0.705(1)	0.8163(8)	0.5902(4)	3.6(3)
Cl(3)	0.4624(8)	0.7590(7)	0.9293(3)	2.0(3)
P(1)	0.7251(8)	1.0761(7)	0.8234(4)	1.5(3)
P(2)	0.7455(8)	0.7736(7)	0.7626(4)	1.4(2)
P(3)	0.4611(8)	0.8162(7)	0.7026(3)	1.8(3)
C(1)	0.677(3)	0.976(2)	0.888(1)	1.1(9)
C(2)	0.605(3)	1.178(2)	0.822(1)	1(1)
C(3)	0.537(4)	1.195(3)	0.758(2)	3(1)
C(4)	0.444(3)	1.271(3)	0.757(2)	2(1)
C(5)	0.437(3)	1.341(3)	0.822(2)	3(1)
C(6)	0.511(3)	1.330(3)	0.890(1)	3(1)
C(7)	0.597(3)	1.251(3)	0.889(1)	3(1)
C(8)	0.900(3)	1.211(3)	0.865(2)	2(1)
C(9)	0.937(3)	1.335(2)	0.842(1)	2(1)
C(10)	1.078(4)	1.444(3)	0.877(2)	3(1)
C(11)	1.182(3)	1.429(4)	0.930(2)	4(1)
C(12)	1.137(3)	1.310(3)	0.956(2)	3(1)
C(13)	1.004(3)	1.208(3)	0.924(1)	3(1)
C(14)	0.617(3)	0.710(2)	0.819(1)	2(1)
C(15)	0.934(3)	0.853(2)	0.821(1)	1(1)
C(16)	0.978(3)	0.793(2)	0.875(1)	2(1)
C(17)	1.120(3)	0.846(3)	0.916(1)	2(1)
C(18)	1.225(3)	0.957(3)	0.906(2)	3(1)
C(19)	1.183(3)	1.020(3)	0.850(1)	2(1)
C(20)	1.037(4)	0.966(3)	0.807(2)	2(1)
C(21)	0.767(3)	0.625(2)	0.698(1)	1(1)
C(22)	0.888(3)	0.645(3)	0.677(2)	3(1)
C(23)	0.903(3)	0.530(3)	0.629(2)	3(1)
C(24)	0.792(4)	0.407(3)	0.603(1)	3(1)
C(25)	0.661(4)	0.392(3)	0.622(1)	4(1)
C(26)	0.636(3)	0.495(2)	0.670(1)	2(1)
C(27)	0.420(3)	0.833(2)	0.791(1)	0.9(9)
C(28)	0.368(3)	0.630(2)	0.657(1)	2(1)
C(29)	0.286(3)	0.535(3)	0.692(1)	2(1)
C(30)	0.204(3)	0.402(3)	0.653(2)	4(1)
C(31)	0.211(5)	0.359(3)	0.583(2)	5(2)
C(32)	0.276(6)	0.441(4)	0.545(2)	8(2)
C(33)	0.364(4)	0.587(3)	0.581(2)	6(2)
C(34)	0.351(3)	0.883(3)	0.641(1)	2(1)
C(35)	0.393(3)	0.909(3)	0.577(1)	2(1)
C(36)	0.309(4)	0.960(3)	0.532(1)	3(1)
C(37)	0.176(3)	0.977(3)	0.550(2)	3(1)
C(38)	0.143(3)	0.950(3)	0.615(2)	4(1)
C(39)	0.228(3)	0.905(3)	0.660(1)	2(1)
B(1)	0.548(3)	0.826(3)	0.852(2)	1.7(6)

Table 22. Intramolecular Distances for **13**.

atom	atom	distance	atom	atom	distance
Ir(1)	Cl(1)	2.331(7)	C(11)	C(12)	1.41(4)
Ir(1)	Cl(2)	2.369(7)	C(12)	C(13)	1.37(3)
Ir(1)	P(1)	2.337(7)	C(14)	B(1)	1.67(4)
Ir(1)	P(2)	2.277(7)	C(15)	C(16)	1.39(3)
Ir(1)	P(3)	2.255(8)	C(15)	C(20)	1.43(3)
Cl(3)	B(1)	1.93(3)	C(16)	C(17)	1.35(3)
P(1)	C(1)	1.79(2)	C(17)	C(18)	1.36(3)
P(1)	C(2)	1.85(2)	C(18)	C(19)	1.43(3)
P(1)	C(8)	1.81(3)	C(19)	C(20)	1.38(3)
P(2)	C(14)	1.83(2)	C(21)	C(22)	1.28(3)
P(2)	C(15)	1.83(2)	C(21)	C(26)	1.48(3)
P(2)	C(21)	1.89(2)	C(22)	C(23)	1.44(4)
P(3)	C(27)	1.78(2)	C(23)	C(24)	1.36(3)
P(3)	C(28)	1.86(2)	C(24)	C(25)	1.34(4)
P(3)	C(34)	1.85(3)	C(25)	C(26)	1.40(3)
C(1)	B(1)	1.62(3)	C(27)	B(1)	1.61(4)
C(2)	C(3)	1.36(3)	C(28)	C(29)	1.38(3)
C(2)	C(7)	1.41(3)	C(28)	C(33)	1.44(4)
C(3)	C(4)	1.40(3)	C(29)	C(30)	1.39(4)
C(4)	C(5)	1.33(3)	C(30)	C(31)	1.35(4)
C(5)	C(6)	1.43(3)	C(31)	C(32)	1.26(4)
C(6)	C(7)	1.38(3)	C(32)	C(33)	1.49(4)
C(8)	C(9)	1.41(3)	C(34)	C(35)	1.40(3)
C(8)	C(13)	1.42(4)	C(34)	C(39)	1.42(3)
C(9)	C(10)	1.42(3)	C(35)	C(36)	1.42(3)
C(10)	C(11)	1.38(4)	C(36)	C(37)	1.45(4)
C(37)	C(38)	1.36(4)	C(38)	C(39)	1.39(4)

Distances are in angstroms. Estimated standard deviations in the least significant figure are given in parentheses.

Table 23. Intramolecular Bond Angles Involving the Nonhydrogen Atoms for **13**.

atom	atom	atom	angle	atom	atom	atom	angle
Cl(1)	Ir(1)	Cl(2)	83.9(3)	C(27)	P(3)	C(34)	112(1)
Cl(1)	Ir(1)	P(1)	88.2(2)	C(28)	P(3)	C(34)	99(1)
Cl(1)	Ir(1)	P(2)	137.1(3)	P(1)	C(1)	B(1)	115(2)
Cl(1)	Ir(1)	P(3)	137.5(3)	P(1)	C(2)	C(3)	122(2)
Cl(2)	Ir(1)	P(1)	171.8(3)	P(1)	C(2)	C(7)	119(2)
Cl(2)	Ir(1)	P(2)	93.4(2)	C(3)	C(2)	C(7)	118(2)
Cl(2)	Ir(1)	P(3)	96.5(3)	C(2)	C(3)	C(4)	122(2)
P(1)	Ir(1)	P(2)	91.0(2)	C(3)	C(4)	C(5)	119(2)
P(1)	Ir(1)	P(3)	90.7(2)	C(4)	C(5)	C(6)	122(3)
P(2)	Ir(1)	P(3)	85.4(2)	C(5)	C(6)	C(7)	118(3)
Ir(1)	P(1)	C(1)	110.6(8)	C(2)	C(7)	C(6)	121(2)
Ir(1)	P(1)	C(2)	114.2(8)	P(1)	C(8)	C(9)	119(2)
Ir(1)	P(1)	C(8)	116.8(9)	P(1)	C(8)	C(13)	123(2)
C(1)	P(1)	C(2)	106(1)	C(9)	C(8)	C(13)	119(2)
C(1)	P(1)	C(8)	108(1)	C(8)	C(9)	C(10)	117(2)
C(2)	P(1)	C(8)	100(1)	C(9)	C(10)	C(11)	124(3)
Ir(1)	P(2)	C(14)	114.1(8)	C(10)	C(11)	C(12)	117(3)
Ir(1)	P(2)	C(15)	107.9(8)	C(11)	C(12)	C(13)	120(3)
Ir(1)	P(2)	C(21)	114.8(7)	C(8)	C(13)	C(12)	122(3)
C(14)	P(2)	C(15)	108(1)	P(2)	C(14)	B(1)	112(2)
C(14)	P(2)	C(21)	111(1)	P(2)	C(15)	C(16)	121(2)
C(15)	P(2)	C(21)	99(1)	P(2)	C(15)	C(20)	120(2)
Ir(1)	P(3)	C(27)	112.2(8)	C(16)	C(15)	C(20)	118(2)
Ir(1)	P(3)	C(28)	122.7(8)	C(15)	C(16)	C(17)	122(2)
Ir(1)	P(3)	C(34)	106.2(9)	C(16)	C(17)	C(18)	121(2)
C(27)	P(3)	C(28)	104(1)	C(17)	C(18)	C(19)	118(3)
C(18)	C(19)	C(20)	121(2)	C(34)	C(39)	C(38)	121(2)
C(15)	C(20)	C(19)	118(2)	Cl(3)	B(1)	C(1)	109(2)
P(2)	C(21)	C(22)	120(2)	Cl(3)	B(1)	C(14)	104(2)
P(2)	C(21)	C(26)	117(2)	Cl(3)	B(1)	C(27)	110(2)
C(22)	C(21)	C(26)	124(2)	C(1)	B(1)	C(14)	110(2)
C(21)	C(22)	C(23)	119(3)	C(1)	B(1)	C(27)	111(2)
C(22)	C(23)	C(24)	120(3)	C(14)	B(1)	C(27)	112(2)
C(23)	C(24)	C(25)	120(3)	C(24)	C(25)	C(26)	124(3)
C(21)	C(26)	C(25)	113(2)	P(3)	C(27)	B(1)	113(2)
P(3)	C(28)	C(29)	123(2)	P(3)	C(28)	C(33)	115(2)
C(29)	C(28)	C(33)	122(2)	C(28)	C(29)	C(30)	121(3)
C(29)	C(30)	C(31)	117(3)	C(30)	C(31)	C(32)	126(3)
C(31)	C(32)	C(33)	122(4)	C(28)	C(33)	C(32)	113(3)
P(3)	C(34)	C(35)	121(2)	P(3)	C(34)	C(39)	119(2)
C(35)	C(34)	C(39)	119(2)	C(34)	C(35)	C(36)	119(2)
C(35)	C(36)	C(37)	120(2)	C(36)	C(37)	C(38)	119(3)
C(37)	C(38)	C(39)	122(3)				

Angles are in degrees. Estimated standard deviations in the least significant figure are given in parentheses.

Table 24. Anistropic displacement parameters for **13**.

atom	U11	U22	U33	U12	U13	U23
Ir(1)	0.040(1)	0.0184(7)	0.0113(6)	0.0181(6)	0.0080(5)	0.0062(5)
Cl(1)	0.071(7)	0.051(6)	0.021(4)	-0.001(5)	0.018(4)	0.018(4)
Cl(2)	0.089(7)	0.047(5)	0.022(4)	0.047(5)	0.023(4)	0.012(4)
Cl(3)	0.034(5)	0.026(4)	0.020(4)	0.011(4)	0.011(3)	0.012(3)
P(1)	0.026(5)	0.009(4)	0.022(4)	0.003(4)	0.012(4)	0.010(3)
P(2)	0.021(5)	0.019(4)	0.015(4)	0.009(4)	0.005(3)	0.006(3)
P(3)	0.044(6)	0.018(4)	0.011(4)	0.020(4)	0.009(4)	-0.000(3)
C(1)	0.01(2)	0.00(1)	0.02(1)	-0.00(1)	-0.00(1)	-0.00(1)
C(2)	0.03(2)	0.02(2)	0.01(1)	0.03(1)	0.03(1)	0.01(1)
C(3)	0.04(3)	0.02(2)	0.03(2)	-0.02(2)	0.01(2)	0.01(1)
C(4)	0.03(2)	0.04(2)	0.04(2)	0.02(2)	0.03(2)	0.02(2)
C(5)	0.04(2)	0.03(2)	0.08(3)	0.03(2)	0.05(2)	0.04(2)
C(6)	0.05(2)	0.02(2)	0.03(2)	-0.01(2)	-0.00(2)	0.02(1)
C(7)	0.07(3)	0.03(2)	0.02(2)	0.04(2)	0.00(2)	0.01(1)
C(8)	-0.02(1)	0.04(2)	0.04(2)	-0.00(1)	0.01(1)	0.03(2)
C(9)	0.02(2)	0.01(2)	0.04(2)	-0.01(1)	0.01(1)	0.02(1)
C(10)	0.06(3)	0.01(2)	0.07(2)	0.03(2)	0.03(2)	0.01(2)
C(11)	0.02(2)	0.08(3)	0.05(2)	0.01(2)	0.02(2)	0.01(2)
C(12)	0.03(2)	0.03(2)	0.04(2)	-0.01(2)	0.02(2)	0.02(2)
C(13)	0.01(2)	0.03(2)	0.04(2)	-0.00(2)	0.01(2)	-0.00(1)
C(14)	0.04(2)	-0.01(1)	0.04(2)	-0.00(1)	0.01(1)	0.02(1)
C(15)	0.02(2)	0.00(1)	0.02(1)	-0.00(1)	0.00(1)	0.01(1)
C(16)	0.01(2)	0.01(2)	0.04(2)	-0.00(1)	0.02(1)	0.01(1)
C(17)	0.03(2)	0.02(2)	0.02(2)	0.00(2)	0.02(1)	0.00(1)
C(18)	0.04(2)	0.05(2)	0.03(2)	0.02(2)	0.01(2)	-0.01(2)
C(19)	0.05(2)	0.02(2)	0.03(2)	0.01(2)	0.03(2)	0.01(1)
C(20)	0.04(2)	0.03(2)	0.02(2)	0.02(2)	0.04(2)	-0.01(2)
C(21)	0.01(2)	0.01(2)	0.03(2)	0.01(1)	-0.01(1)	0.00(1)
C(22)	0.02(2)	0.04(2)	0.03(2)	-0.01(2)	0.02(2)	0.00(2)
C(23)	0.02(2)	0.07(2)	0.03(2)	0.03(2)	-0.01(2)	0.02(2)
C(24)	0.07(3)	0.01(2)	0.02(2)	-0.01(2)	0.00(2)	0.00(1)
C(25)	0.10(3)	0.01(2)	0.01(2)	0.00(2)	0.01(2)	-0.01(1)
C(26)	0.04(2)	0.00(2)	0.04(2)	-0.00(1)	0.01(2)	0.02(1)
C(27)	0.01(2)	0.01(1)	0.02(1)	0.01(1)	0.01(1)	0.01(1)
C(28)	0.03(2)	0.00(1)	0.02(2)	0.01(1)	-0.01(1)	-0.00(1)
C(29)	0.01(2)	0.01(2)	0.03(2)	0.00(1)	-0.01(1)	-0.02(1)

Table 25. Positional parameters and B(eq) for **16**.

atom	x	y	z	B(eq)
Ir(1)	0.06206(5)	0.10232(7)	0.16821(3)	1.45(2)
P(1)	0.1810(3)	0.1229(4)	0.2701(2)	1.5(1)
P(2)	-0.1040(3)	0.1453(4)	0.2189(1)	1.3(1)
P(3)	-0.0532(3)	-0.1241(4)	0.1798(2)	1.6(1)
C(1)	-0.023(1)	0.101(2)	0.0770(7)	2.5(3)
C(2)	0.220(1)	0.265(2)	0.1363(7)	2.3(3)
C(3)	0.063(1)	0.092(1)	0.3350(5)	0.8(2)
C(4)	0.272(1)	0.004(1)	0.2762(6)	1.2(2)
C(5)	0.320(1)	-0.042(1)	0.2217(6)	1.8(3)
C(6)	0.389(1)	-0.134(2)	0.2242(6)	2.0(3)
C(7)	0.414(1)	-0.169(2)	0.2843(7)	2.5(3)
C(8)	0.367(1)	-0.122(2)	0.3387(7)	2.3(3)
C(9)	0.297(1)	-0.035(1)	0.3352(6)	2.0(3)
C(10)	0.323(1)	0.280(1)	0.2937(6)	1.5(2)
C(11)	0.445(1)	0.305(2)	0.2612(6)	2.0(3)
C(12)	0.555(1)	0.427(2)	0.2790(7)	2.2(3)
C(13)	0.546(1)	0.523(2)	0.3270(7)	2.6(3)
C(14)	0.428(1)	0.499(2)	0.3587(7)	2.4(3)
C(15)	0.320(1)	0.380(1)	0.3432(6)	1.7(2)
C(16)	-0.185(1)	0.031(1)	0.2764(6)	1.6(2)
C(17)	-0.239(1)	0.159(1)	0.1648(5)	0.8(2)
C(18)	-0.337(1)	0.046(1)	0.1355(6)	1.6(2)
C(19)	-0.443(1)	0.048(2)	0.0925(6)	2.2(3)
C(20)	-0.440(1)	0.179(2)	0.0820(6)	2.0(3)
C(21)	-0.340(1)	0.294(2)	0.1109(7)	2.6(3)
C(22)	-0.236(1)	0.286(2)	0.1515(6)	2.2(3)
C(23)	-0.048(1)	0.313(1)	0.2649(6)	1.3(2)
C(24)	0.075(1)	0.410(2)	0.2547(7)	2.6(3)
C(25)	0.113(1)	0.539(2)	0.2857(7)	2.7(3)
C(26)	0.029(1)	0.571(2)	0.3273(7)	2.4(3)
C(27)	-0.090(1)	0.482(2)	0.3398(7)	2.8(3)
C(28)	-0.131(1)	0.349(2)	0.3090(7)	2.6(3)
C(29)	-0.060(1)	-0.156(1)	0.2640(5)	0.9(2)
C(30)	0.038(1)	-0.221(1)	0.1347(6)	1.5(2)
C(31)	0.115(1)	-0.169(2)	0.0822(6)	2.0(3)
C(32)	0.174(1)	-0.243(2)	0.0451(7)	2.3(3)
C(33)	0.160(1)	-0.372(2)	0.0586(7)	2.8(3)
C(34)	0.085(1)	-0.426(2)	0.1105(8)	3.6(3)
C(35)	0.028(1)	-0.345(2)	0.1488(7)	2.6(3)
C(36)	-0.221(1)	-0.223(1)	0.1415(6)	1.8(3)
C(37)	-0.239(1)	-0.241(2)	0.0744(6)	2.2(3)
C(38)	-0.367(1)	-0.318(2)	0.0423(7)	2.8(3)
C(39)	-0.475(1)	-0.378(2)	0.0776(8)	3.3(3)
C(40)	-0.457(1)	-0.360(2)	0.1459(7)	2.3(3)
C(41)	-0.336(1)	-0.287(2)	0.1764(6)	2.1(3)
C(42)	-0.151(1)	-0.099(2)	0.3780(6)	1.9(3)
C(43)	-0.075(1)	-0.136(1)	0.4236(6)	1.9(3)
C(44)	-0.131(1)	-0.192(2)	0.4789(7)	2.4(3)
C(45)	-0.264(1)	-0.211(1)	0.4918(6)	1.7(2)
C(46)	-0.341(1)	-0.175(1)	0.4483(6)	1.9(3)
C(47)	-0.285(1)	-0.119(2)	0.3928(6)	2.2(3)
C(48)	0.668(1)	0.410(2)	0.4696(7)	2.8(3)
C(49)	0.787(1)	0.434(2)	0.5080(7)	3.1(3)
C(50)	0.835(1)	0.330(2)	0.5086(7)	3.0(3)

C(51)	0.768(1)	0.205(2)	0.4750(8)	3.3(3)
C(52)	0.645(1)	0.184(2)	0.4372(7)	2.7(3)
C(53)	0.598(1)	0.289(2)	0.4347(7)	2.6(3)
B(1)	-0.083(1)	-0.034(2)	0.3131(7)	1.8(3)

Table 26. Intramolecular Distances Involving the Nonhydrogen Atoms for **16**.

atom	atom	distance	atom	atom	distance
Ir(1)	P(1)	2.390(3)	C(14)	C(15)	1.38(2)
Ir(1)	P(2)	2.218(3)	C(16)	B(1)	1.68(2)
Ir(1)	P(3)	2.326(4)	C(17)	C(18)	1.36(2)
Ir(1)	C(1)	2.08(1)	C(17)	C(22)	1.40(2)
Ir(1)	C(2)	2.11(1)	C(18)	C(19)	1.42(2)
P(1)	C(3)	1.82(1)	C(19)	C(20)	1.42(2)
P(1)	C(4)	1.85(1)	C(20)	C(21)	1.38(2)
P(1)	C(10)	1.82(1)	C(21)	C(22)	1.40(2)
P(2)	C(16)	1.80(1)	C(23)	C(24)	1.38(2)
P(2)	C(17)	1.85(1)	C(23)	C(28)	1.40(2)
P(2)	C(23)	1.83(1)	C(24)	C(25)	1.38(2)
P(3)	C(29)	1.81(1)	C(25)	C(26)	1.35(2)
P(3)	C(30)	1.84(1)	C(26)	C(27)	1.33(2)
P(3)	C(36)	1.83(1)	C(27)	C(28)	1.40(2)
C(3)	B(1)	1.67(2)	C(29)	B(1)	1.66(2)
C(4)	C(5)	1.36(2)	C(30)	C(31)	1.41(2)
C(4)	C(9)	1.38(2)	C(30)	C(35)	1.35(2)
C(5)	C(6)	1.41(2)	C(31)	C(32)	1.36(2)
C(6)	C(7)	1.38(2)	C(32)	C(33)	1.39(2)
C(7)	C(8)	1.36(2)	C(33)	C(34)	1.39(2)
C(8)	C(9)	1.38(2)	C(34)	C(35)	1.42(2)
C(10)	C(11)	1.42(2)	C(36)	C(37)	1.39(2)
C(10)	C(15)	1.42(2)	C(36)	C(41)	1.41(2)
C(11)	C(12)	1.41(2)	C(37)	C(38)	1.41(2)
C(12)	C(13)	1.38(2)	C(38)	C(39)	1.36(2)
C(13)	C(14)	1.37(2)	C(39)	C(40)	1.41(2)
C(40)	C(41)	1.34(2)	C(42)	C(43)	1.40(2)
C(42)	C(47)	1.40(2)	C(42)	B(1)	1.63(2)
C(43)	C(44)	1.39(2)	C(44)	C(45)	1.38(2)
C(45)	C(46)	1.38(2)	C(46)	C(47)	1.40(2)
C(48)	C(49)	1.41(2)	C(48)	C(53)	1.36(2)
C(49)	C(50)	1.37(2)	C(50)	C(51)	1.37(2)
C(51)	C(52)	1.44(2)	C(52)	C(53)	1.37(2)

Distances are in angstroms. Estimated standard deviations in the least significant figure are given in parentheses.

Table 27. Intramolecular Bond Angles Involving the Nonhydrogen Atoms for **16**.

atom	atom	atom	angle	atom	atom	atom	angle
P(1)	Ir(1)	P(2)	90.2(1)	C(29)	P(3)	C(36)	106.4(6)
P(1)	Ir(1)	P(3)	88.2(1)	C(30)	P(3)	C(36)	96.1(6)
P(1)	Ir(1)	C(1)	173.9(4)	P(1)	C(3)	B(1)	112.8(8)
P(1)	Ir(1)	C(2)	92.6(4)	P(1)	C(4)	C(5)	119.4(9)
P(2)	Ir(1)	P(3)	87.2(1)	P(1)	C(4)	C(9)	121.5(9)
P(2)	Ir(1)	C(1)	92.9(4)	C(5)	C(4)	C(9)	119(1)
P(2)	Ir(1)	C(2)	118.5(4)	C(4)	C(5)	C(6)	121(1)
P(3)	Ir(1)	C(1)	97.2(4)	C(5)	C(6)	C(7)	118(1)
P(3)	Ir(1)	C(2)	154.3(4)	C(6)	C(7)	C(8)	121(1)
C(1)	Ir(1)	C(2)	81.3(5)	C(7)	C(8)	C(9)	120(1)
Ir(1)	P(1)	C(3)	110.5(4)	C(4)	C(9)	C(8)	121(1)
Ir(1)	P(1)	C(4)	115.6(4)	P(1)	C(10)	C(11)	119(1)
Ir(1)	P(1)	C(10)	117.1(4)	P(1)	C(10)	C(15)	123.9(9)
C(3)	P(1)	C(4)	105.2(5)	C(11)	C(10)	C(15)	117(1)
C(3)	P(1)	C(10)	109.1(6)	C(10)	C(11)	C(12)	119(1)
C(4)	P(1)	C(10)	98.2(5)	C(11)	C(12)	C(13)	121(1)
Ir(1)	P(2)	C(16)	115.2(4)	C(12)	C(13)	C(14)	120(1)
Ir(1)	P(2)	C(17)	114.9(4)	C(13)	C(14)	C(15)	121(1)
Ir(1)	P(2)	C(23)	113.0(4)	C(10)	C(15)	C(14)	122(1)
C(16)	P(2)	C(17)	107.9(5)	P(2)	C(16)	B(1)	114.9(8)
C(16)	P(2)	C(23)	104.9(6)	P(2)	C(17)	C(18)	120.3(9)
C(17)	P(2)	C(23)	99.4(6)	P(2)	C(17)	C(22)	120(1)
Ir(1)	P(3)	C(29)	112.1(4)	C(18)	C(17)	C(22)	119(1)
Ir(1)	P(3)	C(30)	106.9(4)	C(17)	C(18)	C(19)	124(1)
Ir(1)	P(3)	C(36)	123.7(4)	C(18)	C(19)	C(20)	115(1)
C(29)	P(3)	C(30)	110.1(5)	C(19)	C(20)	C(21)	121(1)
C(20)	C(21)	C(22)	121(1)	C(36)	C(41)	C(40)	121(1)
C(17)	C(22)	C(21)	119(1)	C(43)	C(42)	C(47)	115(1)
P(2)	C(23)	C(24)	121(1)	C(43)	C(42)	B(1)	121(1)
P(2)	C(23)	C(28)	121(1)	C(47)	C(42)	B(1)	123(1)
C(24)	C(23)	C(28)	118(1)	C(42)	C(43)	C(44)	122(1)
C(23)	C(24)	C(25)	121(1)	C(43)	C(44)	C(45)	121(1)
C(24)	C(25)	C(26)	120(1)	C(44)	C(45)	C(46)	119(1)
C(25)	C(26)	C(27)	123(2)	C(45)	C(46)	C(47)	120(1)
C(26)	C(27)	C(28)	119(1)	C(42)	C(47)	C(46)	123(1)
C(23)	C(28)	C(27)	120(1)	C(49)	C(48)	C(53)	123(1)
P(3)	C(29)	B(1)	113.2(9)	C(48)	C(49)	C(50)	118(2)
P(3)	C(30)	C(31)	121(1)	C(49)	C(50)	C(51)	122(1)
P(3)	C(30)	C(35)	121.4(9)	C(50)	C(51)	C(52)	119(1)
C(31)	C(30)	C(35)	118(1)	C(51)	C(52)	C(53)	120(2)
C(30)	C(31)	C(32)	122(1)	C(48)	C(53)	C(52)	119(1)
C(31)	C(32)	C(33)	120(1)	C(3)	B(1)	C(16)	108(1)
C(32)	C(33)	C(34)	121(1)	C(3)	B(1)	C(29)	111.2(9)
C(33)	C(34)	C(35)	118(2)	C(3)	B(1)	C(42)	109(1)
C(30)	C(35)	C(34)	122(1)	C(16)	B(1)	C(29)	111(1)
P(3)	C(36)	C(37)	119.2(9)	C(16)	B(1)	C(42)	111(1)
P(3)	C(36)	C(41)	124(1)	C(29)	B(1)	C(42)	108(1)
C(37)	C(36)	C(41)	117(1)	C(36)	C(37)	C(38)	121(1)
C(37)	C(38)	C(39)	120(1)	C(38)	C(39)	C(40)	119(1)
C(39)	C(40)	C(41)	121(1)				

Angles are in degrees. Estimated standard deviations in the least significant figure are given in parentheses.

Table 28. Anisotropic displacement parameters for **16**.

atom	U11	U22	U33	U12	U13	U23
Ir(1)	0.0224(3)	0.0276(5)	0.0110(3)	0.0139(3)	0.0019(2)	0.0107(3)
P(1)	0.023(2)	0.025(3)	0.013(2)	0.012(2)	-0.000(1)	0.006(2)
P(2)	0.020(2)	0.022(3)	0.009(2)	0.008(2)	-0.002(1)	0.006(2)
P(3)	0.024(2)	0.029(3)	0.011(2)	0.013(2)	0.001(1)	0.010(2)